# Full wwPDB NMR Structure Validation Report (i)

Mar 12, 2026 – 04:25 PM UTC

| | | |
|---|---|---|
| PDB ID | : | 2MBS / pdb_00002mbs |
| BMRB ID | : | 19413 |
| Title | : | NMR solution structure of oxidized KpDsbA |
| Authors | : | Kurth, F.; Rimmer, K.; Premkumar, L.; Mohanty, B.; Duprez, W.; Halili, M.A.; Shouldice, S.R.; Heras, B.; Fairlie, D.P.; Scanlon, M.J.; Martin, J.L. |
| Deposited on | : | 2013-08-03 |

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

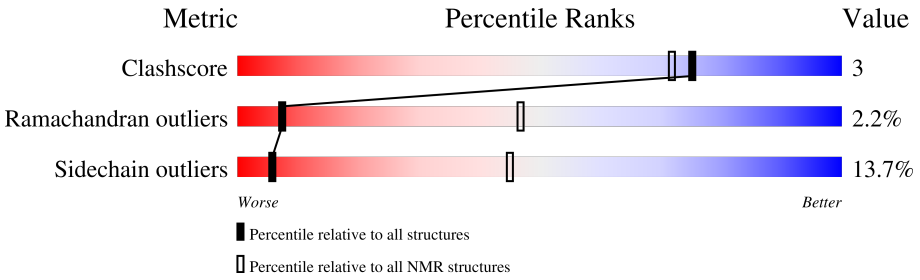
| | | |
|---|---|---|
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| wwPDB-RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| wwPDB-ShiftChecker | : | v1.2 |
| BMRB Restraints Analysis | : | v1.2 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.49 |

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 80%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | NMR archive (#Entries) |
|---|---|---|
| Clashscore | 229148 | 14424 |
| Ramachandran outliers | 224038 | 12848 |
| Sidechain outliers | 223484 | 12823 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 190 | 84% 12% . |

# 2 Ensemble composition and analysis

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues | | | |
|---|---|---|---|
| **Well-defined core** | **Residue range (total)** | **Backbone RMSD (Å)** | **Medoid model** |
| 1 | A:1-A:15, A:22-A:188 (182) | 0.82 | 9 |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 3 single-model clusters were found.

| Cluster number | Models |
|---|---|
| 1 | 2, 4, 5, 7, 8, 9, 10, 13, 15, 16, 19 |
| 2 | 1, 6, 11, 12, 17, 20 |
| Single-model clusters | 3; 14; 18 |

# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2955 atoms, of which 1467 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Thiol:disulfide interchange protein.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 190 | 2955 | 952 | 1467 | 243 | 286 | 7 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -1 | SER | - | expression tag | UNP B5XZJ6 |
| A | 0 | ASN | - | expression tag | UNP B5XZJ6 |

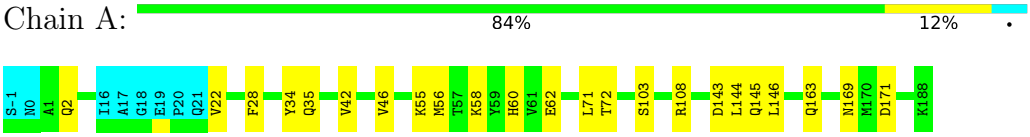
# 4 Residue-property plots

## 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Thiol:disulfide interchange protein

Chain A:



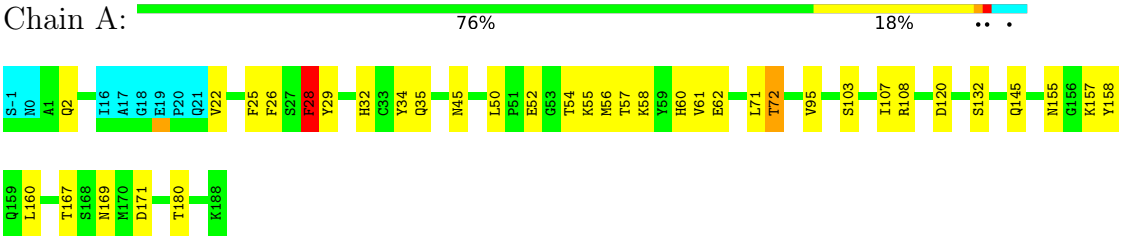

## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

• Molecule 1: Thiol:disulfide interchange protein

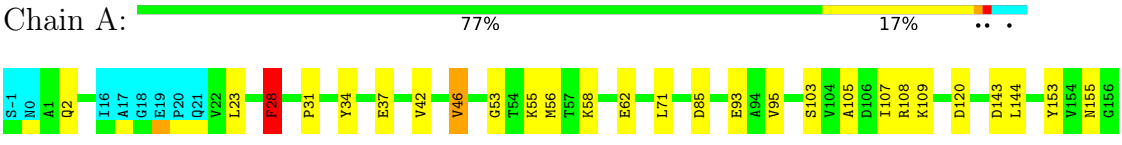
Chain A:




### 4.2.2 Score per residue for model 2

• Molecule 1: Thiol:disulfide interchange protein

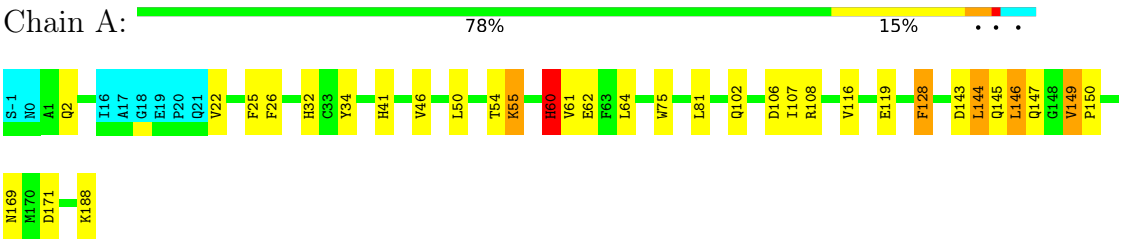
Chain A:



### 4.2.3 Score per residue for model 3

• Molecule 1: Thiol:disulfide interchange protein

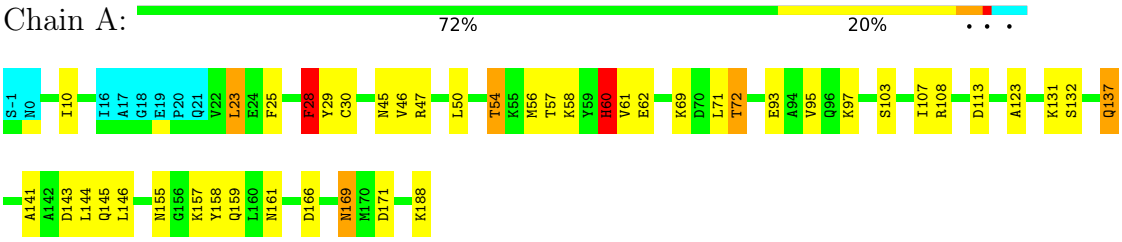
Chain A:




### 4.2.4 Score per residue for model 4

• Molecule 1: Thiol:disulfide interchange protein

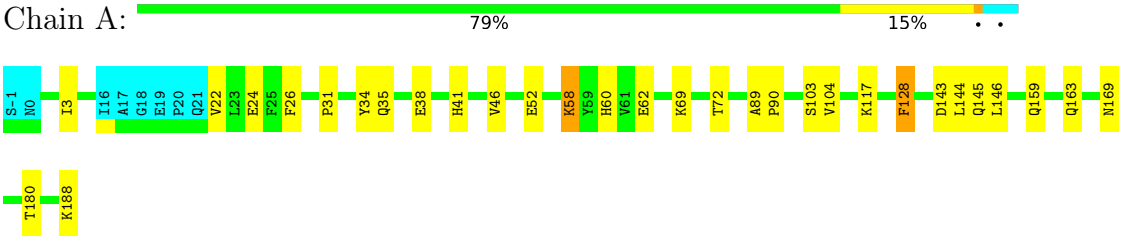
Chain A:




### 4.2.5 Score per residue for model 5

• Molecule 1: Thiol:disulfide interchange protein

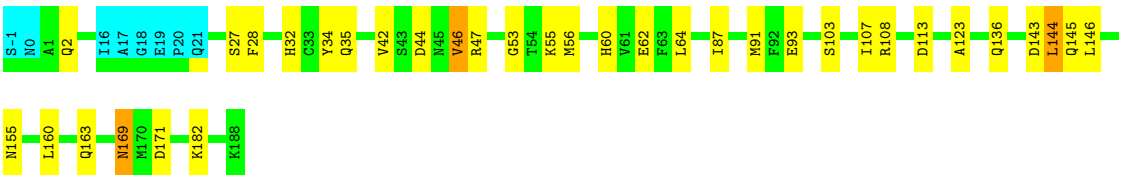
Chain A:




### 4.2.6 Score per residue for model 6

• Molecule 1: Thiol:disulfide interchange protein

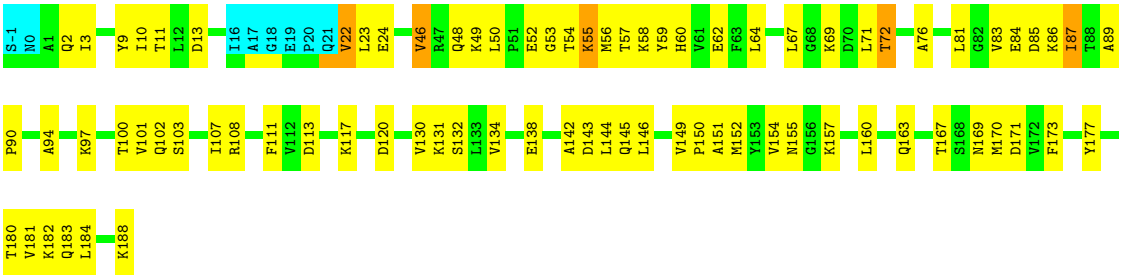
Chain A:




### 4.2.7 Score per residue for model 7

• Molecule 1: Thiol:disulfide interchange protein

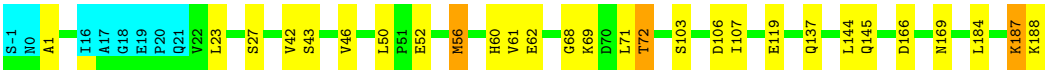
Chain A:




### 4.2.8 Score per residue for model 8

• Molecule 1: Thiol:disulfide interchange protein

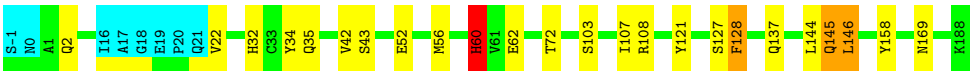
Chain A:




### 4.2.9 Score per residue for model 9 (medoid)

• Molecule 1: Thiol:disulfide interchange protein

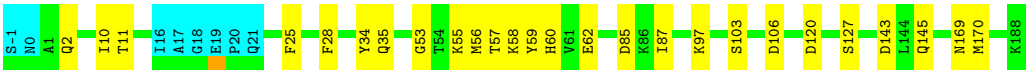
Chain A:




### 4.2.10 Score per residue for model 10

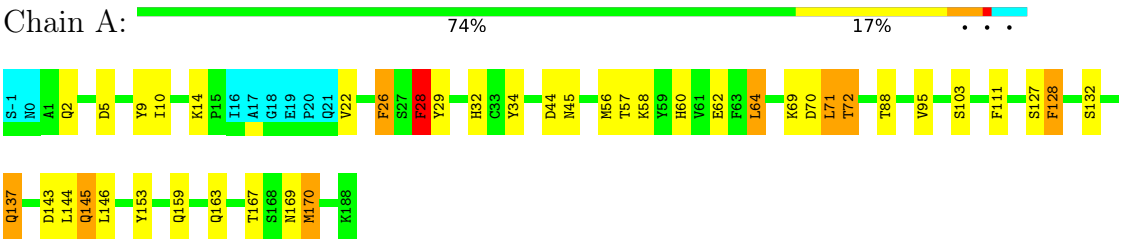
• Molecule 1: Thiol:disulfide interchange protein

Chain A:



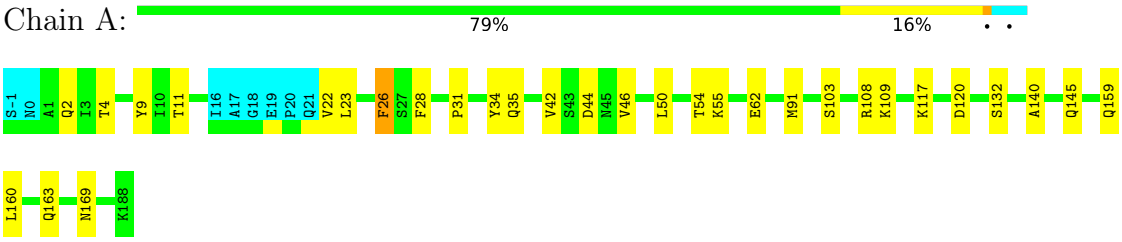

### 4.2.11 Score per residue for model 11

• Molecule 1: Thiol:disulfide interchange protein



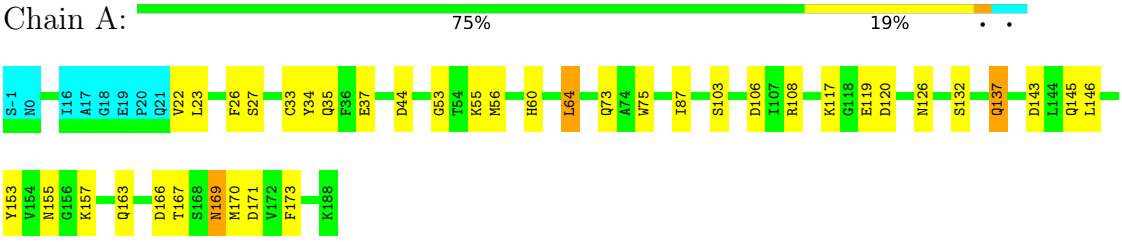

### 4.2.12 Score per residue for model 12

• Molecule 1: Thiol:disulfide interchange protein



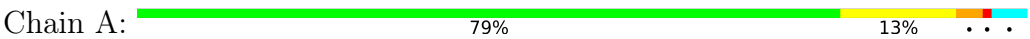

### 4.2.13 Score per residue for model 13

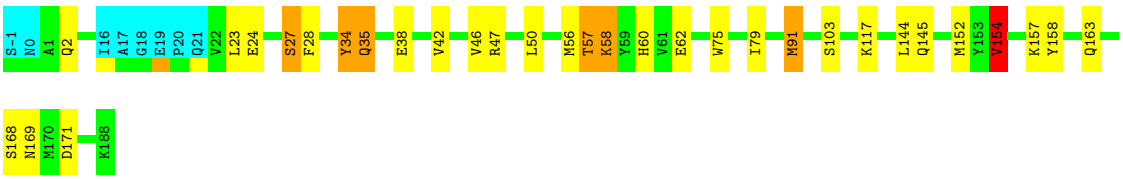
• Molecule 1: Thiol:disulfide interchange protein




### 4.2.14 Score per residue for model 14

• Molecule 1: Thiol:disulfide interchange protein

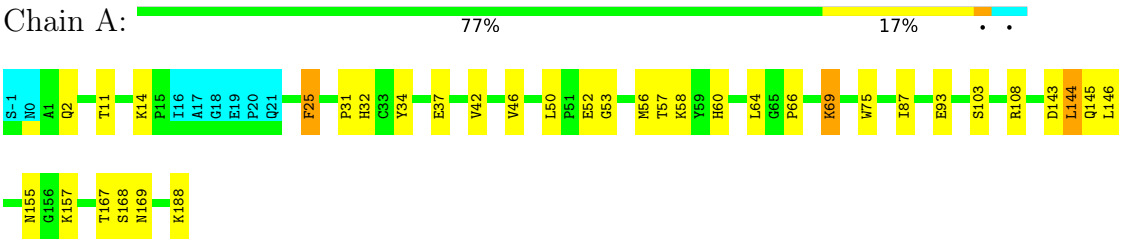





### 4.2.15 Score per residue for model 15

• Molecule 1: Thiol:disulfide interchange protein

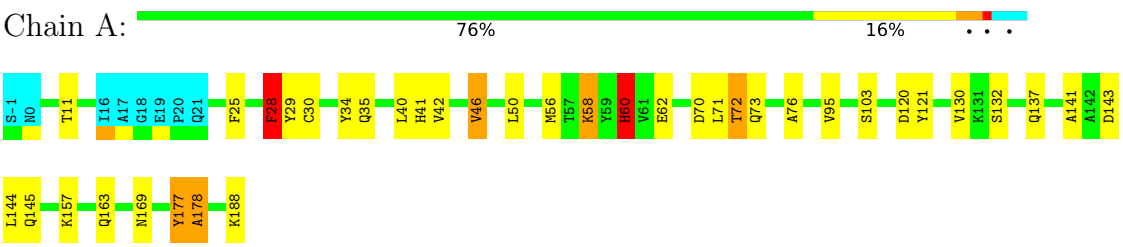
Chain A:




### 4.2.16 Score per residue for model 16

• Molecule 1: Thiol:disulfide interchange protein

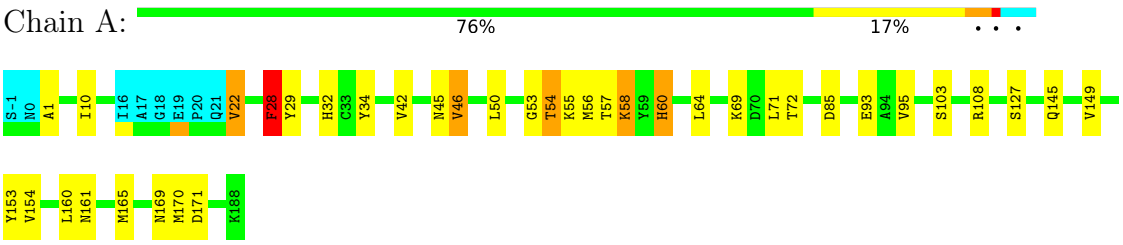
Chain A:




### 4.2.17 Score per residue for model 17

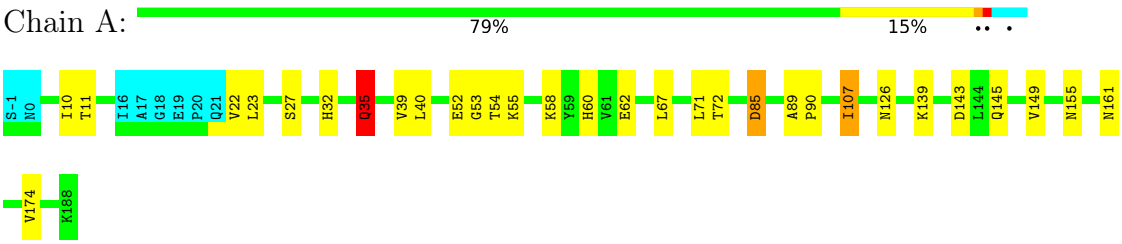
• Molecule 1: Thiol:disulfide interchange protein

Chain A:



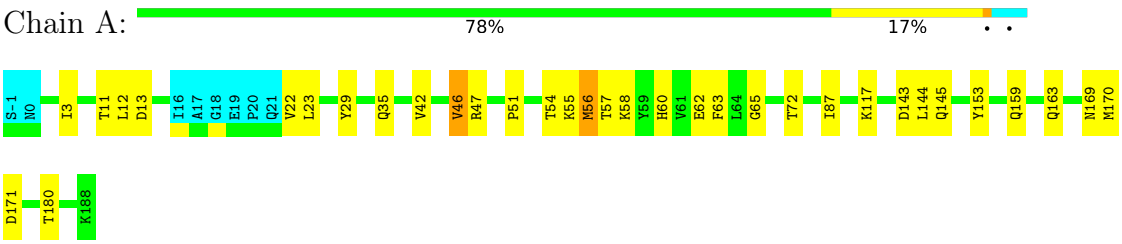

### 4.2.18 Score per residue for model 18

• Molecule 1: Thiol:disulfide interchange protein



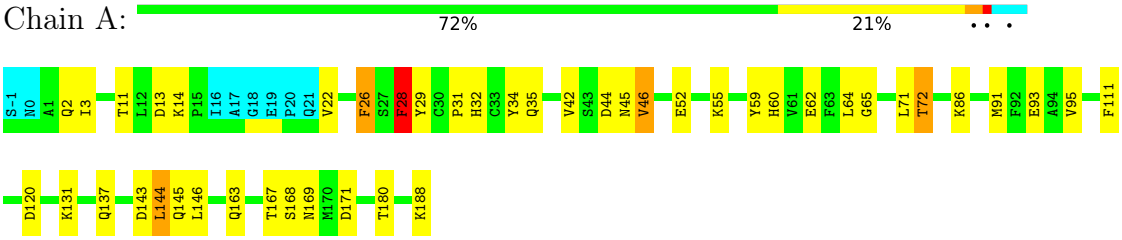

### 4.2.19 Score per residue for model 19

• Molecule 1: Thiol:disulfide interchange protein




### 4.2.20 Score per residue for model 20

• Molecule 1: Thiol:disulfide interchange protein



# 5 Refinement protocol and experimental data overview

The models were refined using the following method: *water refinement*.

Of the 40 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---|---|---|
| CYANA | structure solution | 3.0 |
| OPALp | refinement | |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| Chemical shift file(s) | working_cs.cif |
|---|---|
| Number of chemical shift lists | 1 |
| Total number of shifts | 2023 |
| Number of shifts mapped to atoms | 2023 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 80% |

# 6 Model quality

## 6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 0.62±0.09 | 0±0/1462 ( 0.0± 0.0%) | 1.36±0.16 | 4±3/1982 ( 0.2± 0.1%) |
| All | All | 0.63 | 1/29240 ( 0.0%) | 1.37 | 90/39640 ( 0.2%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | Chirality | Planarity |
|---|---|---|---|
| 1 | A | 0.0±0.0 | 1.9±1.1 |
| All | All | 0 | 37 |

All unique bond outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 178 | ALA | CA-C | 5.57 | 1.60 | 1.52 | 16 | 1 |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 28 | PHE | CA-CB-CG | 14.19 | 127.99 | 113.80 | 16 | 7 |
| 1 | A | 154 | VAL | CA-CB-CG1 | 13.00 | 132.49 | 110.40 | 14 | 1 |
| 1 | A | 25 | PHE | CA-CB-CG | 9.01 | 122.81 | 113.80 | 15 | 2 |
| 1 | A | 39 | VAL | CB-CA-C | 7.90 | 118.65 | 110.91 | 18 | 1 |
| 1 | A | 26 | PHE | CA-CB-CG | 7.65 | 121.45 | 113.80 | 12 | 3 |
| 1 | A | 39 | VAL | N-CA-C | -7.53 | 105.80 | 112.12 | 18 | 1 |
| 1 | A | 128 | PHE | N-CA-C | 6.99 | 119.75 | 111.71 | 11 | 3 |
| 1 | A | 71 | LEU | CA-C-N | 6.97 | 129.51 | 120.44 | 18 | 2 |
| 1 | A | 71 | LEU | C-N-CA | 6.97 | 129.51 | 120.44 | 18 | 2 |
| 1 | A | 12 | LEU | CA-C-N | 6.40 | 129.38 | 120.29 | 19 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 12 | LEU | C-N-CA | 6.40 | 129.38 | 120.29 | 19 | 1 |
| 1 | A | 32 | HIS | CB-CG-CD2 | -6.16 | 123.20 | 131.20 | 11 | 9 |
| 1 | A | 85 | ASP | CA-CB-CG | 6.04 | 118.64 | 112.60 | 18 | 2 |
| 1 | A | 50 | LEU | CA-C-N | 6.01 | 127.36 | 119.84 | 15 | 1 |
| 1 | A | 50 | LEU | C-N-CA | 6.01 | 127.36 | 119.84 | 15 | 1 |
| 1 | A | 30 | CYS | CB-CA-C | 5.92 | 116.92 | 108.68 | 16 | 2 |
| 1 | A | 2 | GLN | CA-C-N | 5.83 | 130.97 | 122.69 | 10 | 1 |
| 1 | A | 2 | GLN | C-N-CA | 5.83 | 130.97 | 122.69 | 10 | 1 |
| 1 | A | 144 | LEU | CA-C-N | 5.78 | 129.85 | 120.60 | 9 | 1 |
| 1 | A | 144 | LEU | C-N-CA | 5.78 | 129.85 | 120.60 | 9 | 1 |
| 1 | A | 60 | HIS | CB-CG-CD2 | -5.71 | 123.78 | 131.20 | 3 | 3 |
| 1 | A | 65 | GLY | CA-C-N | 5.59 | 124.94 | 118.85 | 20 | 1 |
| 1 | A | 65 | GLY | C-N-CA | 5.59 | 124.94 | 118.85 | 20 | 1 |
| 1 | A | 13 | ASP | CA-CB-CG | 5.55 | 118.15 | 112.60 | 19 | 1 |
| 1 | A | 169 | ASN | CA-CB-CG | 5.52 | 118.12 | 112.60 | 13 | 2 |
| 1 | A | 127 | SER | CA-C-N | 5.48 | 128.18 | 120.28 | 17 | 4 |
| 1 | A | 127 | SER | C-N-CA | 5.48 | 128.18 | 120.28 | 17 | 4 |
| 1 | A | 128 | PHE | CA-CB-CG | 5.41 | 119.21 | 113.80 | 5 | 1 |
| 1 | A | 33 | CYS | CA-C-N | 5.33 | 128.20 | 120.79 | 13 | 1 |
| 1 | A | 33 | CYS | C-N-CA | 5.33 | 128.20 | 120.79 | 13 | 1 |
| 1 | A | 60 | HIS | N-CA-CB | -5.33 | 102.19 | 110.46 | 16 | 1 |
| 1 | A | 143 | ASP | CA-C-N | 5.31 | 131.68 | 121.54 | 19 | 1 |
| 1 | A | 143 | ASP | C-N-CA | 5.31 | 131.68 | 121.54 | 19 | 1 |
| 1 | A | 169 | ASN | CA-C-N | 5.24 | 131.54 | 121.54 | 6 | 1 |
| 1 | A | 169 | ASN | C-N-CA | 5.24 | 131.54 | 121.54 | 6 | 1 |
| 1 | A | 4 | THR | CA-C-N | 5.22 | 131.52 | 121.54 | 12 | 1 |
| 1 | A | 4 | THR | C-N-CA | 5.22 | 131.52 | 121.54 | 12 | 1 |
| 1 | A | 111 | PHE | CA-CB-CG | 5.19 | 118.99 | 113.80 | 11 | 1 |
| 1 | A | 43 | SER | N-CA-CB | -5.18 | 102.29 | 110.06 | 9 | 1 |
| 1 | A | 104 | VAL | CA-C-N | 5.16 | 127.44 | 120.38 | 5 | 1 |
| 1 | A | 104 | VAL | C-N-CA | 5.16 | 127.44 | 120.38 | 5 | 1 |
| 1 | A | 69 | LYS | CA-C-N | 5.13 | 127.11 | 120.44 | 15 | 1 |
| 1 | A | 69 | LYS | C-N-CA | 5.13 | 127.11 | 120.44 | 15 | 1 |
| 1 | A | 120 | ASP | CA-CB-CG | -5.12 | 107.48 | 112.60 | 10 | 1 |
| 1 | A | 123 | ALA | CA-C-N | 5.12 | 127.40 | 120.38 | 4 | 2 |
| 1 | A | 123 | ALA | C-N-CA | 5.12 | 127.40 | 120.38 | 4 | 2 |
| 1 | A | 120 | ASP | N-CA-C | -5.11 | 105.79 | 111.36 | 12 | 1 |
| 1 | A | 167 | THR | CB-CA-C | 5.09 | 120.55 | 110.42 | 1 | 1 |
| 1 | A | 128 | PHE | CA-C-N | 5.08 | 127.42 | 120.77 | 3 | 1 |
| 1 | A | 128 | PHE | C-N-CA | 5.08 | 127.42 | 120.77 | 3 | 1 |
| 1 | A | 42 | VAL | CA-C-N | 5.07 | 127.33 | 120.38 | 9 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 42 | VAL | C-N-CA | 5.07 | 127.33 | 120.38 | 9 | 1 |
| 1 | A | 163 | GLN | N-CA-CB | -5.07 | 102.50 | 110.46 | 6 | 1 |
| 1 | A | 35 | GLN | CB-CG-CD | 5.07 | 121.21 | 112.60 | 18 | 1 |
| 1 | A | 161 | ASN | CA-CB-CG | -5.05 | 107.55 | 112.60 | 4 | 1 |
| 1 | A | 88 | THR | CB-CA-C | 5.04 | 117.15 | 109.34 | 11 | 1 |

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Group | Models (Total) |
|---|---|---|---|---|---|
| 1 | A | 34 | TYR | Sidechain | 15 |
| 1 | A | 29 | TYR | Sidechain | 6 |
| 1 | A | 153 | TYR | Sidechain | 5 |
| 1 | A | 121 | TYR | Sidechain | 2 |
| 1 | A | 25 | PHE | Sidechain | 2 |
| 1 | A | 47 | ARG | Sidechain | 1 |
| 1 | A | 158 | TYR | Sidechain | 1 |
| 1 | A | 59 | TYR | Sidechain | 1 |
| 1 | A | 9 | TYR | Sidechain | 1 |
| 1 | A | 140 | ALA | Peptide | 1 |
| 1 | A | 177 | TYR | Sidechain | 1 |
| 1 | A | 54 | THR | Peptide | 1 |

## 6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|---|---|---|---|---|---|
| 1 | A | 1432 | 1416 | 1416 | 9±8 |
| All | All | 28640 | 28320 | 28320 | 179 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:28:PHE:CD1 | 1:A:71:LEU:HD11 | 0.76 | 2.16 | 4 | 6 |
| 1:A:25:PHE:CE1 | 1:A:149:VAL:HG13 | 0.75 | 2.17 | 3 | 1 |
| 1:A:28:PHE:CD2 | 1:A:95:VAL:HG21 | 0.75 | 2.16 | 4 | 6 |
| 1:A:28:PHE:CZ | 1:A:71:LEU:HD21 | 0.74 | 2.16 | 11 | 4 |
| 1:A:60:HIS:CE1 | 1:A:72:THR:HG22 | 0.74 | 2.17 | 7 | 6 |
| 1:A:25:PHE:CD1 | 1:A:149:VAL:HG13 | 0.68 | 2.24 | 3 | 1 |
| 1:A:23:LEU:HD11 | 1:A:59:TYR:CD1 | 0.65 | 2.25 | 7 | 1 |
| 1:A:89:ALA:HB3 | 1:A:90:PRO:HD3 | 0.64 | 1.68 | 7 | 3 |
| 1:A:24:GLU:CD | 1:A:152:MET:HE2 | 0.64 | 2.18 | 7 | 1 |
| 1:A:25:PHE:CE2 | 1:A:61:VAL:HG21 | 0.64 | 2.28 | 3 | 1 |
| 1:A:3:ILE:HD12 | 1:A:9:TYR:CE2 | 0.64 | 2.28 | 7 | 1 |
| 1:A:67:LEU:HD11 | 1:A:102:GLN:O | 0.63 | 1.93 | 7 | 1 |
| 1:A:9:TYR:O | 1:A:10:ILE:HD13 | 0.62 | 1.93 | 7 | 2 |
| 1:A:24:GLU:OE1 | 1:A:152:MET:HE2 | 0.61 | 1.94 | 7 | 1 |
| 1:A:60:HIS:H | 1:A:60:HIS:CD2 | 0.61 | 2.13 | 13 | 1 |
| 1:A:28:PHE:CE1 | 1:A:71:LEU:HD11 | 0.60 | 2.31 | 4 | 4 |
| 1:A:87:ILE:HD13 | 1:A:111:PHE:CZ | 0.60 | 2.30 | 7 | 1 |
| 1:A:130:VAL:O | 1:A:134:VAL:HG23 | 0.60 | 1.95 | 7 | 1 |
| 1:A:60:HIS:CE1 | 1:A:72:THR:HG23 | 0.60 | 2.31 | 18 | 4 |
| 1:A:22:VAL:HG21 | 1:A:54:THR:HG23 | 0.60 | 1.72 | 1 | 1 |
| 1:A:154:VAL:HG12 | 1:A:158:TYR:HB2 | 0.60 | 1.74 | 14 | 1 |
| 1:A:89:ALA:HB3 | 1:A:90:PRO:CD | 0.59 | 2.28 | 7 | 1 |
| 1:A:47:ARG:HB2 | 1:A:56:MET:HE1 | 0.58 | 1.75 | 19 | 2 |
| 1:A:50:LEU:HD13 | 1:A:54:THR:O | 0.58 | 1.99 | 4 | 1 |
| 1:A:81:LEU:HD21 | 1:A:120:ASP:CG | 0.57 | 2.24 | 7 | 1 |
| 1:A:60:HIS:CD2 | 1:A:75:TRP:CD1 | 0.57 | 2.92 | 13 | 1 |
| 1:A:10:ILE:HD11 | 1:A:161:ASN:CG | 0.57 | 2.25 | 17 | 1 |
| 1:A:28:PHE:CE2 | 1:A:71:LEU:HD21 | 0.56 | 2.36 | 1 | 6 |
| 1:A:35:GLN:HE21 | 1:A:35:GLN:HA | 0.56 | 1.59 | 18 | 2 |
| 1:A:3:ILE:HD12 | 1:A:9:TYR:CD2 | 0.56 | 2.35 | 7 | 1 |
| 1:A:60:HIS:CE1 | 1:A:72:THR:CG2 | 0.55 | 2.89 | 11 | 4 |
| 1:A:3:ILE:HG21 | 1:A:180:THR:HG23 | 0.55 | 1.78 | 20 | 3 |
| 1:A:76:ALA:CB | 1:A:130:VAL:HG13 | 0.55 | 2.30 | 7 | 1 |
| 1:A:46:VAL:HG12 | 1:A:50:LEU:HG | 0.55 | 1.79 | 7 | 4 |
| 1:A:83:VAL:HG12 | 1:A:86:LYS:HD2 | 0.55 | 1.78 | 7 | 1 |
| 1:A:146:LEU:HD11 | 1:A:151:ALA:CB | 0.54 | 2.32 | 7 | 1 |
| 1:A:154:VAL:HG11 | 1:A:184:LEU:HB2 | 0.54 | 1.80 | 7 | 1 |
| 1:A:76:ALA:HB3 | 1:A:130:VAL:HG13 | 0.53 | 1.79 | 7 | 2 |
| 1:A:167:THR:HG22 | 1:A:173:PHE:CD1 | 0.53 | 2.39 | 7 | 2 |
| 1:A:25:PHE:CE1 | 1:A:141:ALA:HB2 | 0.53 | 2.39 | 16 | 1 |
| 1:A:35:GLN:HB3 | 1:A:40:LEU:HD13 | 0.52 | 1.80 | 18 | 1 |
| 1:A:177:TYR:O | 1:A:181:VAL:HG23 | 0.52 | 2.05 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:24:GLU:OE2 | 1:A:152:MET:HE2 | 0.52 | 2.04 | 14 | 1 |
| 1:A:42:VAL:O | 1:A:46:VAL:HG23 | 0.51 | 2.05 | 12 | 9 |
| 1:A:60:HIS:CE1 | 1:A:137:GLN:CB | 0.51 | 2.93 | 11 | 2 |
| 1:A:60:HIS:CE1 | 1:A:137:GLN:HE21 | 0.51 | 2.22 | 20 | 1 |
| 1:A:40:LEU:O | 1:A:42:VAL:HG23 | 0.51 | 2.05 | 16 | 1 |
| 1:A:184:LEU:HD23 | 1:A:187:LYS:HD3 | 0.50 | 1.83 | 8 | 1 |
| 1:A:117:LYS:HG3 | 1:A:120:ASP:CB | 0.50 | 2.37 | 13 | 1 |
| 1:A:28:PHE:CD2 | 1:A:60:HIS:CE1 | 0.50 | 3.00 | 6 | 2 |
| 1:A:170:MET:HA | 1:A:170:MET:HE2 | 0.50 | 1.84 | 7 | 1 |
| 1:A:50:LEU:HD13 | 1:A:54:THR:HG21 | 0.50 | 1.82 | 12 | 3 |
| 1:A:101:VAL:HG13 | 1:A:107:ILE:HG12 | 0.50 | 1.82 | 7 | 1 |
| 1:A:67:LEU:HD13 | 1:A:107:ILE:HD11 | 0.50 | 1.82 | 18 | 1 |
| 1:A:61:VAL:HG12 | 1:A:141:ALA:HB1 | 0.49 | 1.84 | 4 | 1 |
| 1:A:94:ALA:HB1 | 1:A:100:THR:HG22 | 0.49 | 1.85 | 7 | 1 |
| 1:A:3:ILE:HG21 | 1:A:180:THR:CB | 0.48 | 2.38 | 7 | 1 |
| 1:A:60:HIS:CD2 | 1:A:75:TRP:HB3 | 0.48 | 2.43 | 15 | 1 |
| 1:A:160:LEU:HD11 | 1:A:180:THR:HG23 | 0.48 | 1.86 | 7 | 2 |
| 1:A:51:PRO:O | 1:A:54:THR:HG22 | 0.48 | 2.08 | 19 | 1 |
| 1:A:50:LEU:HD22 | 1:A:54:THR:HG21 | 0.48 | 1.86 | 1 | 1 |
| 1:A:157:LYS:HE2 | 1:A:158:TYR:CE2 | 0.48 | 2.44 | 1 | 1 |
| 1:A:67:LEU:HD11 | 1:A:102:GLN:C | 0.48 | 2.32 | 7 | 1 |
| 1:A:60:HIS:NE2 | 1:A:72:THR:HG23 | 0.48 | 2.24 | 19 | 1 |
| 1:A:47:ARG:CB | 1:A:56:MET:HE1 | 0.48 | 2.39 | 19 | 1 |
| 1:A:60:HIS:CE1 | 1:A:137:GLN:HB2 | 0.47 | 2.44 | 4 | 1 |
| 1:A:81:LEU:HD12 | 1:A:116:VAL:HG13 | 0.47 | 1.84 | 3 | 1 |
| 1:A:60:HIS:CD2 | 1:A:72:THR:HA | 0.47 | 2.45 | 9 | 1 |
| 1:A:149:VAL:HA | 1:A:150:PRO:C | 0.47 | 2.34 | 7 | 1 |
| 1:A:154:VAL:CG1 | 1:A:158:TYR:HB2 | 0.47 | 2.38 | 14 | 1 |
| 1:A:91:MET:HA | 1:A:91:MET:HE2 | 0.47 | 1.87 | 14 | 1 |
| 1:A:47:ARG:HA | 1:A:50:LEU:HD12 | 0.46 | 1.87 | 4 | 1 |
| 1:A:149:VAL:HG12 | 1:A:150:PRO:HA | 0.46 | 1.86 | 3 | 1 |
| 1:A:9:TYR:C | 1:A:10:ILE:HD13 | 0.46 | 2.35 | 7 | 1 |
| 1:A:28:PHE:CD2 | 1:A:71:LEU:HD21 | 0.46 | 2.45 | 1 | 2 |
| 1:A:154:VAL:HG11 | 1:A:184:LEU:CB | 0.46 | 2.41 | 7 | 1 |
| 1:A:83:VAL:HG12 | 1:A:86:LYS:CD | 0.45 | 2.41 | 7 | 1 |
| 1:A:28:PHE:CE2 | 1:A:95:VAL:HG21 | 0.45 | 2.46 | 4 | 1 |
| 1:A:25:PHE:CD2 | 1:A:146:LEU:HD21 | 0.45 | 2.46 | 3 | 1 |
| 1:A:184:LEU:HD23 | 1:A:187:LYS:CD | 0.45 | 2.41 | 8 | 1 |
| 1:A:60:HIS:CD2 | 1:A:72:THR:HG22 | 0.45 | 2.46 | 20 | 1 |
| 1:A:28:PHE:CZ | 1:A:91:MET:HG3 | 0.45 | 2.47 | 14 | 1 |
| 1:A:50:LEU:HB3 | 1:A:54:THR:HG21 | 0.45 | 1.87 | 17 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:52:GLU:H | 1:A:52:GLU:CD | 0.45 | 2.19 | 8 | 1 |
| 1:A:146:LEU:HD23 | 1:A:147:GLN:H | 0.45 | 1.71 | 3 | 1 |
| 1:A:50:LEU:CD1 | 1:A:56:MET:HE2 | 0.45 | 2.41 | 14 | 1 |
| 1:A:25:PHE:CD2 | 1:A:61:VAL:HG11 | 0.44 | 2.48 | 3 | 1 |
| 1:A:89:ALA:CB | 1:A:90:PRO:CD | 0.44 | 2.94 | 7 | 1 |
| 1:A:117:LYS:HG3 | 1:A:120:ASP:HB2 | 0.44 | 1.89 | 13 | 1 |
| 1:A:46:VAL:O | 1:A:50:LEU:N | 0.43 | 2.51 | 7 | 1 |
| 1:A:87:ILE:HD12 | 1:A:87:ILE:O | 0.43 | 2.13 | 7 | 1 |
| 1:A:94:ALA:HB1 | 1:A:100:THR:CG2 | 0.43 | 2.44 | 7 | 1 |
| 1:A:28:PHE:CE2 | 1:A:91:MET:HG2 | 0.43 | 2.49 | 12 | 1 |
| 1:A:71:LEU:HD23 | 1:A:107:ILE:HG21 | 0.43 | 1.90 | 7 | 1 |
| 1:A:23:LEU:HD22 | 1:A:25:PHE:CZ | 0.43 | 2.49 | 4 | 1 |
| 1:A:75:TRP:CD1 | 1:A:79:ILE:HD11 | 0.43 | 2.48 | 14 | 1 |
| 1:A:60:HIS:O | 1:A:61:VAL:HG13 | 0.43 | 2.14 | 1 | 1 |
| 1:A:46:VAL:HG12 | 1:A:50:LEU:CG | 0.43 | 2.42 | 7 | 1 |
| 1:A:68:GLY:HA2 | 1:A:71:LEU:HD12 | 0.43 | 1.89 | 8 | 1 |
| 1:A:35:GLN:CB | 1:A:40:LEU:HD13 | 0.43 | 2.44 | 18 | 1 |
| 1:A:27:SER:HA | 1:A:60:HIS:CE1 | 0.42 | 2.49 | 6 | 2 |
| 1:A:157:LYS:HE2 | 1:A:158:TYR:CZ | 0.42 | 2.49 | 4 | 1 |
| 1:A:57:THR:HG22 | 1:A:58:LYS:H | 0.42 | 1.75 | 14 | 1 |
| 1:A:26:PHE:HA | 1:A:149:VAL:HG11 | 0.42 | 1.89 | 3 | 1 |
| 1:A:93:GLU:CG | 1:A:97:LYS:HE3 | 0.42 | 2.45 | 4 | 1 |
| 1:A:145:GLN:CD | 1:A:146:LEU:H | 0.42 | 2.23 | 11 | 1 |
| 1:A:29:TYR:CD2 | 1:A:65:GLY:HA3 | 0.42 | 2.50 | 19 | 1 |
| 1:A:91:MET:HE1 | 1:A:111:PHE:CD1 | 0.42 | 2.50 | 20 | 1 |
| 1:A:145:GLN:HE21 | 1:A:146:LEU:N | 0.42 | 2.13 | 9 | 1 |
| 1:A:60:HIS:CD2 | 1:A:72:THR:HG23 | 0.42 | 2.50 | 19 | 1 |
| 1:A:167:THR:O | 1:A:170:MET:HE3 | 0.41 | 2.15 | 11 | 1 |
| 1:A:170:MET:HE2 | 1:A:170:MET:HA | 0.41 | 1.90 | 11 | 1 |
| 1:A:60:HIS:HB2 | 1:A:75:TRP:CG | 0.41 | 2.49 | 3 | 1 |
| 1:A:56:MET:HE2 | 1:A:56:MET:H | 0.41 | 1.76 | 8 | 1 |
| 1:A:138:GLU:O | 1:A:142:ALA:HB3 | 0.41 | 2.16 | 7 | 1 |
| 1:A:28:PHE:CD1 | 1:A:95:VAL:HG11 | 0.41 | 2.51 | 16 | 1 |
| 1:A:89:ALA:N | 1:A:90:PRO:HD2 | 0.41 | 2.30 | 7 | 1 |
| 1:A:60:HIS:CD2 | 1:A:137:GLN:HG2 | 0.41 | 2.51 | 13 | 1 |
| 1:A:46:VAL:O | 1:A:49:LYS:N | 0.40 | 2.54 | 7 | 1 |
| 1:A:59:TYR:CD2 | 1:A:137:GLN:HG3 | 0.40 | 2.51 | 20 | 1 |

## 6.3 Torsion angles (i)

### 6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 181/190 (95%) | 154±4 (85±2%) | 23±3 (13±2%) | 4±2 (2±1%) | 7 47 |
| All | All | 3620/3800 (95%) | 3081 (85%) | 458 (13%) | 81 (2%) | 7 47 |

All 24 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 55 | LYS | 12 |
| 1 | A | 144 | LEU | 10 |
| 1 | A | 143 | ASP | 9 |
| 1 | A | 22 | VAL | 9 |
| 1 | A | 53 | GLY | 8 |
| 1 | A | 31 | PRO | 5 |
| 1 | A | 64 | LEU | 5 |
| 1 | A | 58 | LYS | 4 |
| 1 | A | 157 | LYS | 3 |
| 1 | A | 1 | ALA | 2 |
| 1 | A | 105 | ALA | 1 |
| 1 | A | 54 | THR | 1 |
| 1 | A | 97 | LYS | 1 |
| 1 | A | 56 | MET | 1 |
| 1 | A | 155 | ASN | 1 |
| 1 | A | 57 | THR | 1 |
| 1 | A | 66 | PRO | 1 |
| 1 | A | 167 | THR | 1 |
| 1 | A | 41 | HIS | 1 |
| 1 | A | 177 | TYR | 1 |
| 1 | A | 178 | ALA | 1 |
| 1 | A | 154 | VAL | 1 |
| 1 | A | 63 | PHE | 1 |
| 1 | A | 146 | LEU | 1 |

### 6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 154/160 (96%) | 133±4 (86±2%) | 21±4 (14±2%) | 6 45 |
| All | All | 3080/3200 (96%) | 2659 (86%) | 421 (14%) | 6 45 |

All 85 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 145 | GLN | 19 |
| 1 | A | 169 | ASN | 19 |
| 1 | A | 62 | GLU | 17 |
| 1 | A | 103 | SER | 16 |
| 1 | A | 35 | GLN | 12 |
| 1 | A | 56 | MET | 12 |
| 1 | A | 58 | LYS | 12 |
| 1 | A | 2 | GLN | 11 |
| 1 | A | 108 | ARG | 11 |
| 1 | A | 171 | ASP | 11 |
| 1 | A | 163 | GLN | 10 |
| 1 | A | 46 | VAL | 9 |
| 1 | A | 188 | LYS | 9 |
| 1 | A | 28 | PHE | 8 |
| 1 | A | 57 | THR | 8 |
| 1 | A | 72 | THR | 8 |
| 1 | A | 107 | ILE | 8 |
| 1 | A | 23 | LEU | 8 |
| 1 | A | 11 | THR | 8 |
| 1 | A | 52 | GLU | 7 |
| 1 | A | 132 | SER | 7 |
| 1 | A | 155 | ASN | 7 |
| 1 | A | 60 | HIS | 7 |
| 1 | A | 144 | LEU | 7 |
| 1 | A | 146 | LEU | 7 |
| 1 | A | 69 | LYS | 7 |
| 1 | A | 26 | PHE | 6 |
| 1 | A | 87 | ILE | 6 |
| 1 | A | 45 | ASN | 5 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 93 | GLU | 5 |
| 1 | A | 64 | LEU | 5 |
| 1 | A | 137 | GLN | 5 |
| 1 | A | 159 | GLN | 5 |
| 1 | A | 117 | LYS | 5 |
| 1 | A | 44 | ASP | 5 |
| 1 | A | 170 | MET | 5 |
| 1 | A | 120 | ASP | 4 |
| 1 | A | 85 | ASP | 4 |
| 1 | A | 160 | LEU | 4 |
| 1 | A | 166 | ASP | 4 |
| 1 | A | 106 | ASP | 4 |
| 1 | A | 128 | PHE | 4 |
| 1 | A | 27 | SER | 4 |
| 1 | A | 143 | ASP | 4 |
| 1 | A | 37 | GLU | 3 |
| 1 | A | 182 | LYS | 3 |
| 1 | A | 119 | GLU | 3 |
| 1 | A | 149 | VAL | 3 |
| 1 | A | 10 | ILE | 3 |
| 1 | A | 113 | ASP | 3 |
| 1 | A | 131 | LYS | 3 |
| 1 | A | 157 | LYS | 3 |
| 1 | A | 14 | LYS | 3 |
| 1 | A | 22 | VAL | 3 |
| 1 | A | 168 | SER | 3 |
| 1 | A | 109 | LYS | 2 |
| 1 | A | 41 | HIS | 2 |
| 1 | A | 55 | LYS | 2 |
| 1 | A | 38 | GLU | 2 |
| 1 | A | 91 | MET | 2 |
| 1 | A | 13 | ASP | 2 |
| 1 | A | 70 | ASP | 2 |
| 1 | A | 73 | GLN | 2 |
| 1 | A | 126 | ASN | 2 |
| 1 | A | 102 | GLN | 1 |
| 1 | A | 24 | GLU | 1 |
| 1 | A | 136 | GLN | 1 |
| 1 | A | 48 | GLN | 1 |
| 1 | A | 84 | GLU | 1 |
| 1 | A | 183 | GLN | 1 |
| 1 | A | 43 | SER | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 61 | VAL | 1 |
| 1 | A | 187 | LYS | 1 |
| 1 | A | 97 | LYS | 1 |
| 1 | A | 5 | ASP | 1 |
| 1 | A | 34 | TYR | 1 |
| 1 | A | 47 | ARG | 1 |
| 1 | A | 154 | VAL | 1 |
| 1 | A | 54 | THR | 1 |
| 1 | A | 165 | MET | 1 |
| 1 | A | 139 | LYS | 1 |
| 1 | A | 161 | ASN | 1 |
| 1 | A | 174 | VAL | 1 |
| 1 | A | 86 | LYS | 1 |
| 1 | A | 167 | THR | 1 |

#### 6.3.3 RNA

There are no RNA molecules in this entry.

### 6.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.5 Carbohydrates

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry

There are no ligands in this entry.

### 6.7 Other polymers

There are no such molecules in this entry.

### 6.8 Polymer linkage issues

There are no chain breaks in this entry.

# 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 79% for the entire structure.

## 7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

| | |
|---|---|
| Total number of shifts | 2023 |
| Number of shifts mapped to atoms | 2023 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 6 |

### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction ± precision, *ppm* | Suggested action |
|---|---|---|---|
| $^{13}C_{\alpha}$ | 185 | -0.31 ± 0.15 | None needed (< 0.5 ppm) |
| $^{13}C_{\beta}$ | 175 | 0.22 ± 0.10 | None needed (< 0.5 ppm) |
| $^{13}C'$ | 0 | — | None (insufficient data) |
| $^{15}N$ | 169 | -0.06 ± 0.11 | None needed (< 0.5 ppm) |

### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 1981 atoms were assigned a chemical shift out of a possible 2463. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}H$ | $^{13}C$ | $^{15}N$ |
|---|---|---|---|---|
| Backbone | 706/906 (78%) | 358/367 (98%) | 180/364 (49%) | 168/175 (96%) |
| Sidechain | 1165/1350 (86%) | 796/879 (91%) | 355/428 (83%) | 14/43 (33%) |

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| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Aromatic | 110/207 (53%) | 61/101 (60%) | 47/101 (47%) | 2/5 (40%) |
| Overall | 1981/2463 (80%) | 1215/1347 (90%) | 582/893 (65%) | 184/223 (83%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 2023 atoms were assigned a chemical shift out of a possible 2555. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Backbone | 719/945 (76%) | 365/383 (95%) | 185/380 (49%) | 169/182 (93%) |
| Sidechain | 1194/1403 (85%) | 816/913 (89%) | 364/445 (82%) | 14/45 (31%) |
| Aromatic | 110/207 (53%) | 61/101 (60%) | 47/101 (47%) | 2/5 (40%) |
| Overall | 2023/2555 (79%) | 1242/1397 (89%) | 596/926 (64%) | 185/232 (80%) |

### 7.1.4 Statistically unusual chemical shifts (i)

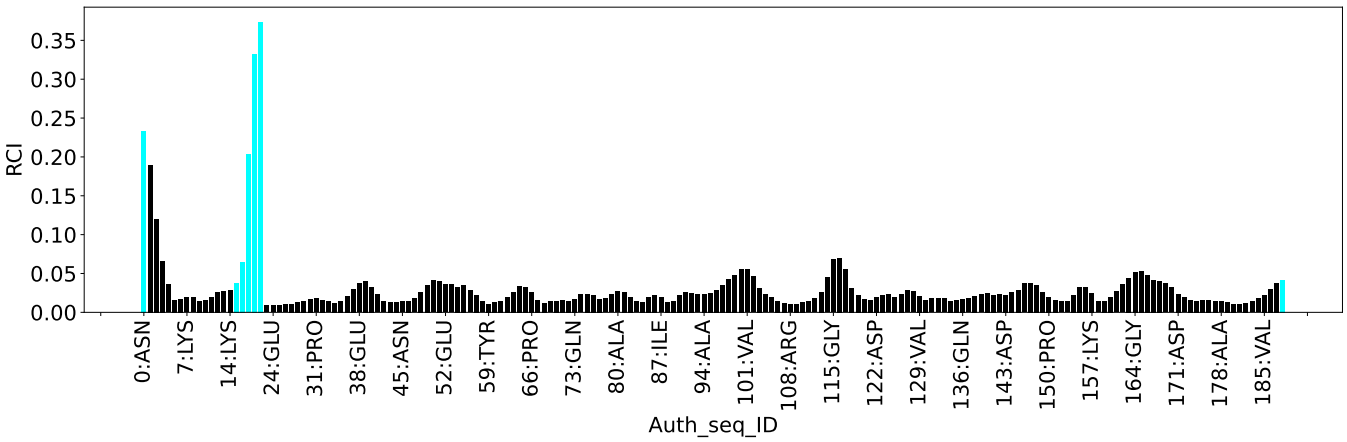
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, *ppm* | Expected range, *ppm* | Z-score |
|---|---|---|---|---|---|---|---|
| 1 | A | 73 | GLN | HG2 | 0.43 | 1.01 – 3.62 | -7.2 |
| 1 | A | 16 | ILE | CG2 | 26.89 | 10.93 – 24.12 | 7.1 |
| 1 | A | 184 | LEU | HD21 | -1.06 | -0.65 – 2.13 | -6.5 |
| 1 | A | 184 | LEU | HD22 | -1.06 | -0.65 – 2.13 | -6.5 |
| 1 | A | 184 | LEU | HD23 | -1.06 | -0.65 – 2.13 | -6.5 |
| 1 | A | 16 | ILE | CG1 | 17.50 | 19.24 – 36.26 | -6.0 |

### 7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0:ASN
7:LYS
14:LYS
24:GLU
31:PRO
38:GLU
45:ASN
52:GLU
59:TYR
66:PRO
73:GLN
80:ALA
87:ILE
94:ALA
101:VAL
108:ARG
115:GLY
122:ASP
129:VAL
136:GLN
143:ASP
150:PRO
157:LYS
164:GLY
171:ASP
178:ALA
185:VAL
Auth_seq_ID

# 8 NMR restraints analysis

## 8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

| Description | Value |
|---|---|
| Total distance restraints | 3531 |
| Intra-residue (\|i-j\|=0) | 733 |
| Sequential (\|i-j\|=1) | 991 |
| Medium range (\|i-j\|>1 and \|i-j\|<5) | 901 |
| Long range (\|i-j\|≥5) | 906 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 0 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 18.6 |
| Number of long range restraints per residue[1] | 4.8 |

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

## 8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

### 8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å
are not included in the calculation.

| Bins (Å) | Average number of violations per model | Max (Å) |
|---|---|---|
| 0.1-0.2 (Small) | 90.8 | 0.2 |
| 0.2-0.5 (Medium) | 148.3 | 0.5 |
| >0.5 (Large) | 288.4 | 5.36 |

### 8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

# 9 Distance violation analysis (i)

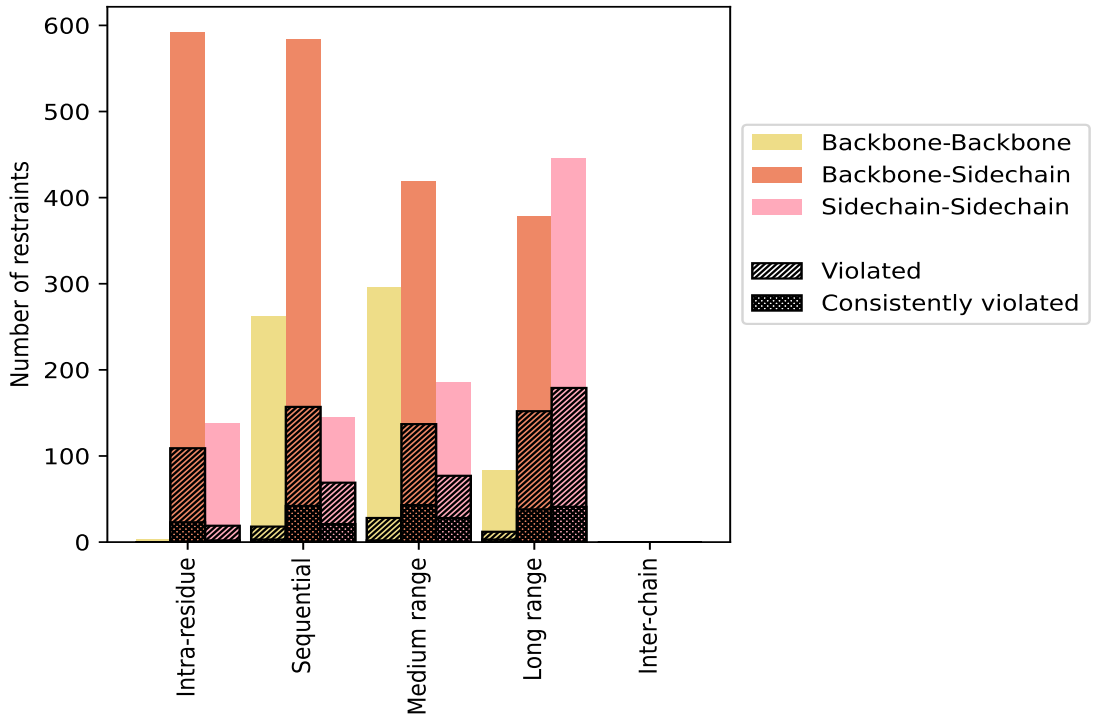
## 9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

| Restraints type | Count | %[1] | Violated[3] | | | Consistently Violated[4] | | |
|---|---|---|---|---|---|---|---|---|
| | | | Count | %[2] | %[1] | Count | %[2] | %[1] |
| Intra-residue (\|i-j\|=0) | 733 | 20.8 | 128 | 17.5 | 3.6 | 25 | 3.4 | 0.7 |
| Backbone-Backbone | 3 | 0.1 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 592 | 16.8 | 109 | 18.4 | 3.1 | 23 | 3.9 | 0.7 |
| Sidechain-Sidechain | 138 | 3.9 | 19 | 13.8 | 0.5 | 2 | 1.4 | 0.1 |
| Sequential (\|i-j\|=1) | 991 | 28.1 | 244 | 24.6 | 6.9 | 66 | 6.7 | 1.9 |
| Backbone-Backbone | 262 | 7.4 | 18 | 6.9 | 0.5 | 3 | 1.1 | 0.1 |
| Backbone-Sidechain | 584 | 16.5 | 157 | 26.9 | 4.4 | 42 | 7.2 | 1.2 |
| Sidechain-Sidechain | 145 | 4.1 | 69 | 47.6 | 2.0 | 21 | 14.5 | 0.6 |
| Medium range (\|i-j\|>1 & \|i-j\|<5) | 901 | 25.5 | 242 | 26.9 | 6.9 | 73 | 8.1 | 2.1 |
| Backbone-Backbone | 296 | 8.4 | 28 | 9.5 | 0.8 | 2 | 0.7 | 0.1 |
| Backbone-Sidechain | 419 | 11.9 | 137 | 32.7 | 3.9 | 43 | 10.3 | 1.2 |
| Sidechain-Sidechain | 186 | 5.3 | 77 | 41.4 | 2.2 | 28 | 15.1 | 0.8 |
| Long range (\|i-j\|≥5) | 906 | 25.7 | 343 | 37.9 | 9.7 | 82 | 9.1 | 2.3 |
| Backbone-Backbone | 83 | 2.4 | 12 | 14.5 | 0.3 | 3 | 3.6 | 0.1 |
| Backbone-Sidechain | 378 | 10.7 | 152 | 40.2 | 4.3 | 38 | 10.1 | 1.1 |
| Sidechain-Sidechain | 445 | 12.6 | 179 | 40.2 | 5.1 | 41 | 9.2 | 1.2 |
| Inter-chain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Hydrogen bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 3531 | 100.0 | 957 | 27.1 | 27.1 | 246 | 7.0 | 7.0 |
| Backbone-Backbone | 644 | 18.2 | 58 | 9.0 | 1.6 | 8 | 1.2 | 0.2 |
| Backbone-Sidechain | 1973 | 55.9 | 555 | 28.1 | 15.7 | 146 | 7.4 | 4.1 |
| Sidechain-Sidechain | 914 | 25.9 | 344 | 37.6 | 9.7 | 92 | 10.1 | 2.6 |

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

### 9.1.1 Bar chart : Distribution of distance restraints and violations




Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

## 9.2 Distance violation statistics for each model

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å
are not included in the statistics.

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD[6] (Å) | Median (Å) |
|---|---|---|---|---|---|---|---|---|---|---|
| | IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | | | | |
| 1 | 72 | 143 | 136 | 197 | 0 | 548 | 0.75 | 4.81 | 0.68 | 0.53 |
| 2 | 77 | 137 | 132 | 189 | 0 | 535 | 0.76 | 4.79 | 0.67 | 0.54 |
| 3 | 74 | 137 | 140 | 187 | 0 | 538 | 0.73 | 4.31 | 0.61 | 0.56 |
| 4 | 70 | 137 | 141 | 180 | 0 | 528 | 0.74 | 4.89 | 0.66 | 0.55 |
| 5 | 67 | 144 | 144 | 194 | 0 | 549 | 0.75 | 4.55 | 0.65 | 0.53 |
| 6 | 71 | 138 | 139 | 188 | 0 | 536 | 0.74 | 4.31 | 0.66 | 0.56 |
| 7 | 65 | 123 | 138 | 185 | 0 | 511 | 0.77 | 5.12 | 0.67 | 0.56 |
| 8 | 75 | 145 | 131 | 177 | 0 | 528 | 0.77 | 4.92 | 0.69 | 0.56 |
| 9 | 74 | 147 | 142 | 184 | 0 | 547 | 0.77 | 5.36 | 0.71 | 0.57 |
| 10 | 66 | 148 | 140 | 195 | 0 | 549 | 0.74 | 3.65 | 0.64 | 0.53 |

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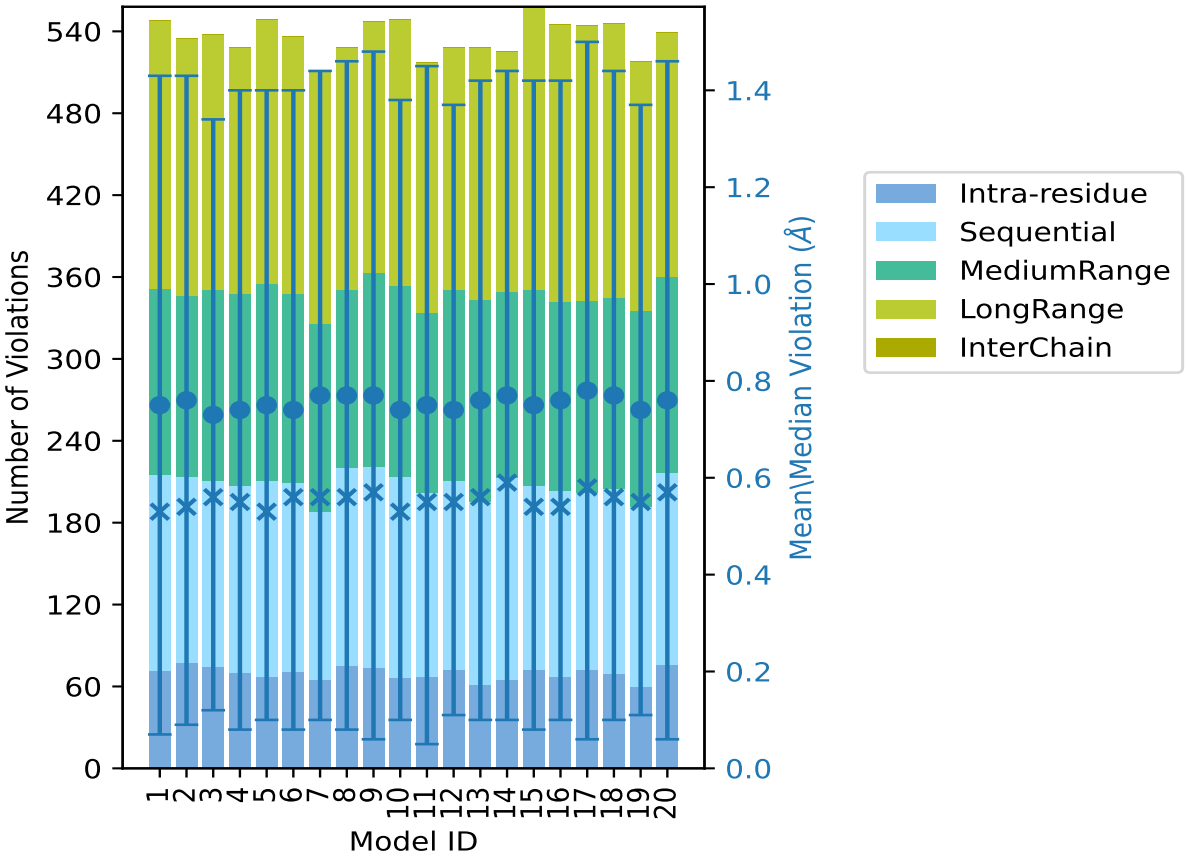
| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD[6] (Å) | Median (Å) |
|---|---|---|---|---|---|---|---|---|---|---|
| | IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | | | | |
| 11 | 67 | 135 | 132 | 183 | 0 | 517 | 0.75 | 5.36 | 0.7 | 0.55 |
| 12 | 72 | 139 | 140 | 177 | 0 | 528 | 0.74 | 4.44 | 0.63 | 0.55 |
| 13 | 61 | 134 | 148 | 185 | 0 | 528 | 0.76 | 4.42 | 0.66 | 0.56 |
| 14 | 65 | 148 | 136 | 176 | 0 | 525 | 0.77 | 4.67 | 0.67 | 0.59 |
| 15 | 72 | 135 | 144 | 207 | 0 | 558 | 0.75 | 5.18 | 0.67 | 0.54 |
| 16 | 67 | 136 | 139 | 203 | 0 | 545 | 0.76 | 3.77 | 0.66 | 0.54 |
| 17 | 72 | 130 | 141 | 201 | 0 | 544 | 0.78 | 5.14 | 0.72 | 0.58 |
| 18 | 69 | 136 | 140 | 201 | 0 | 546 | 0.77 | 4.31 | 0.67 | 0.56 |
| 19 | 60 | 132 | 143 | 183 | 0 | 518 | 0.74 | 4.01 | 0.63 | 0.55 |
| 20 | 76 | 141 | 143 | 179 | 0 | 539 | 0.76 | 4.34 | 0.7 | 0.57 |

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model




The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

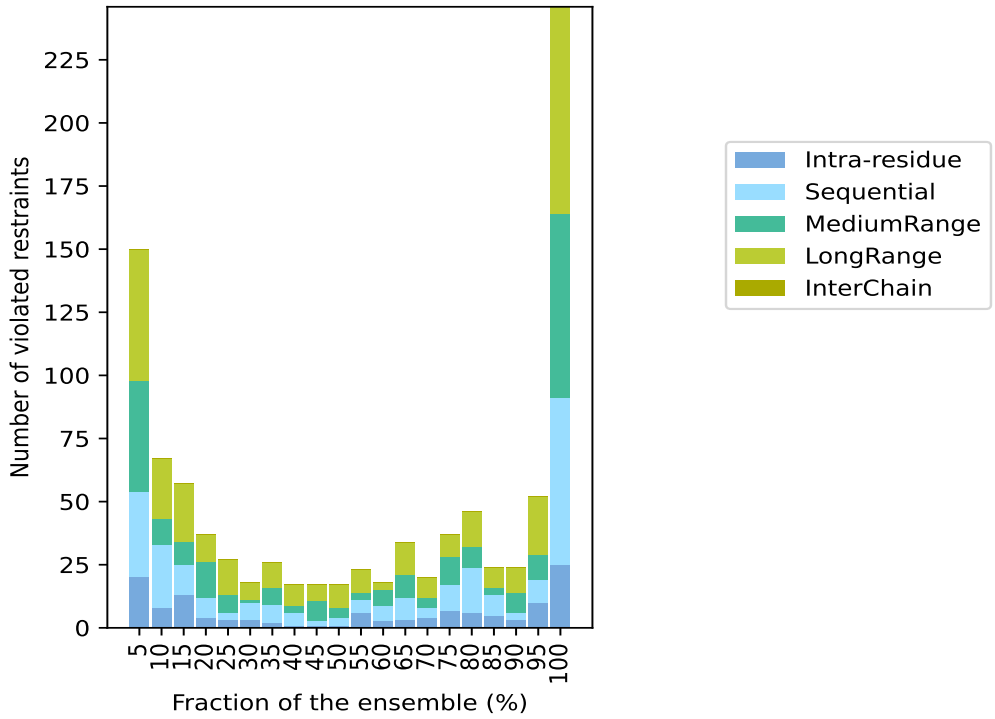
## 9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2574(IR:605, SQ:747, MR:659, LR:563, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints | | | | | | Fraction of the ensemble | |
|---|---|---|---|---|---|---|---|
| IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | Count[6] | % |
| 20 | 34 | 44 | 52 | 0 | 150 | 1 | 5.0 |
| 8 | 25 | 10 | 24 | 0 | 67 | 2 | 10.0 |
| 13 | 12 | 9 | 23 | 0 | 57 | 3 | 15.0 |
| 4 | 8 | 14 | 11 | 0 | 37 | 4 | 20.0 |
| 3 | 3 | 7 | 14 | 0 | 27 | 5 | 25.0 |
| 3 | 7 | 1 | 7 | 0 | 18 | 6 | 30.0 |
| 2 | 7 | 7 | 10 | 0 | 26 | 7 | 35.0 |
| 1 | 5 | 3 | 8 | 0 | 17 | 8 | 40.0 |
| 1 | 2 | 8 | 6 | 0 | 17 | 9 | 45.0 |
| 1 | 3 | 4 | 9 | 0 | 17 | 10 | 50.0 |
| 6 | 5 | 3 | 9 | 0 | 23 | 11 | 55.0 |
| 3 | 6 | 6 | 3 | 0 | 18 | 12 | 60.0 |
| 3 | 9 | 9 | 13 | 0 | 34 | 13 | 65.0 |
| 4 | 4 | 4 | 8 | 0 | 20 | 14 | 70.0 |
| 7 | 10 | 11 | 9 | 0 | 37 | 15 | 75.0 |
| 6 | 18 | 8 | 14 | 0 | 46 | 16 | 80.0 |
| 5 | 8 | 3 | 8 | 0 | 24 | 17 | 85.0 |
| 3 | 3 | 8 | 10 | 0 | 24 | 18 | 90.0 |
| 10 | 9 | 10 | 23 | 0 | 52 | 19 | 95.0 |
| 25 | 66 | 73 | 82 | 0 | 246 | 20 | 100.0 |

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

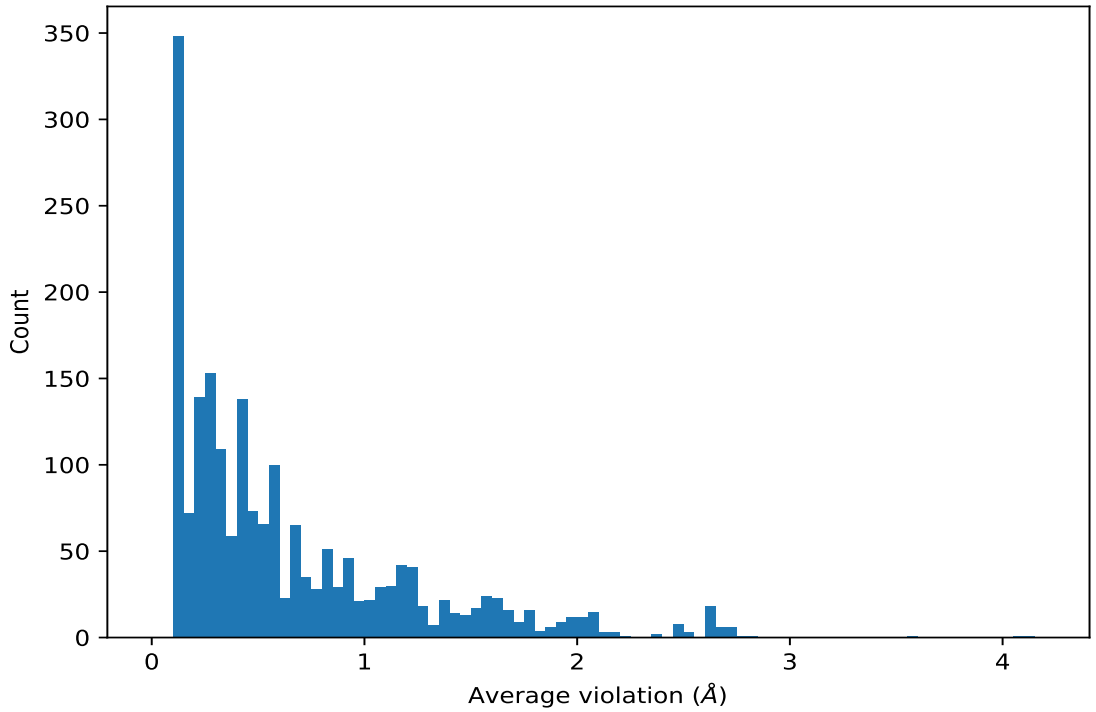
### 9.3.1 Bar graph : Distance violation statistics for the ensemble




## 9.4 Most violated distance restraints in the ensemble

### 9.4.1 Histogram : Distribution of mean distance violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble




### 9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of theviolation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 20 | 4.14 | 0.97 | 4.35 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 20 | 4.06 | 0.6 | 4.11 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 20 | 3.58 | 1.11 | 3.76 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 20 | 2.83 | 0.36 | 2.84 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 20 | 2.77 | 0.84 | 2.64 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 20 | 2.7 | 1.27 | 2.77 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 20 | 2.7 | 1.27 | 2.77 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 20 | 2.7 | 1.27 | 2.77 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 20 | 2.7 | 1.27 | 2.77 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 20 | 2.7 | 1.27 | 2.77 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 20 | 2.7 | 1.27 | 2.77 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 20 | 2.68 | 0.72 | 2.65 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 20 | 2.68 | 0.72 | 2.65 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 20 | 2.68 | 0.72 | 2.65 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 20 | 2.64 | 0.17 | 2.7 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 20 | 2.64 | 0.17 | 2.7 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 20 | 2.64 | 0.17 | 2.7 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 20 | 2.64 | 0.17 | 2.7 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 20 | 2.64 | 0.17 | 2.7 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 20 | 2.64 | 0.17 | 2.7 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 20 | 2.64 | 0.17 | 2.7 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 20 | 2.64 | 0.17 | 2.7 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 20 | 2.64 | 0.17 | 2.7 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 20 | 2.62 | 0.9 | 2.54 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 20 | 2.62 | 0.9 | 2.54 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 20 | 2.62 | 0.9 | 2.54 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 20 | 2.62 | 0.9 | 2.54 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 20 | 2.62 | 0.9 | 2.54 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 20 | 2.62 | 0.9 | 2.54 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 20 | 2.62 | 0.9 | 2.54 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 20 | 2.62 | 0.9 | 2.54 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 20 | 2.62 | 0.9 | 2.54 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 20 | 2.52 | 1.07 | 2.55 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 20 | 2.52 | 1.07 | 2.55 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 20 | 2.52 | 1.07 | 2.55 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 20 | 2.48 | 0.33 | 2.58 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 20 | 2.48 | 0.33 | 2.58 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 20 | 2.48 | 0.33 | 2.58 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 20 | 2.47 | 0.19 | 2.49 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 20 | 2.47 | 0.19 | 2.49 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 20 | 2.47 | 0.19 | 2.49 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 20 | 2.46 | 0.64 | 2.58 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 20 | 2.46 | 0.64 | 2.58 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 20 | 2.39 | 0.69 | 2.39 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 20 | 2.38 | 0.61 | 2.56 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 20 | 2.24 | 0.18 | 2.26 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 20 | 2.19 | 0.06 | 2.21 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 20 | 2.19 | 0.06 | 2.21 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 20 | 2.19 | 0.06 | 2.21 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 20 | 2.11 | 0.15 | 2.12 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 20 | 2.11 | 0.15 | 2.12 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 20 | 2.11 | 0.15 | 2.12 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 20 | 2.09 | 0.16 | 2.08 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 20 | 2.09 | 0.16 | 2.08 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 20 | 2.09 | 0.16 | 2.08 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 20 | 2.08 | 0.25 | 2.12 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 20 | 2.08 | 0.25 | 2.12 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 20 | 2.08 | 0.25 | 2.12 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 20 | 2.07 | 0.15 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 20 | 2.07 | 0.15 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 20 | 2.07 | 0.15 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 20 | 2.07 | 0.15 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 20 | 2.07 | 0.15 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 20 | 2.07 | 0.15 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 20 | 2.07 | 0.15 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 20 | 2.07 | 0.15 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 20 | 2.07 | 0.15 | 2.1 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 20 | 2.01 | 0.71 | 2.01 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 20 | 2.01 | 0.71 | 2.01 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 20 | 2.01 | 0.71 | 2.01 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 20 | 2.0 | 0.15 | 2.04 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 20 | 2.0 | 0.15 | 2.04 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 20 | 2.0 | 0.15 | 2.04 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 20 | 2.0 | 0.19 | 1.98 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 20 | 2.0 | 0.19 | 1.98 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 20 | 2.0 | 0.19 | 1.98 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 20 | 1.99 | 0.29 | 2.05 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 20 | 1.99 | 0.29 | 2.05 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 20 | 1.99 | 0.29 | 2.05 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 20 | 1.98 | 0.68 | 1.94 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 20 | 1.98 | 0.68 | 1.94 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 20 | 1.98 | 0.18 | 1.98 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 20 | 1.98 | 0.18 | 1.98 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 20 | 1.98 | 0.18 | 1.98 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 20 | 1.98 | 0.18 | 1.98 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 20 | 1.98 | 0.18 | 1.98 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 20 | 1.98 | 0.18 | 1.98 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 20 | 1.97 | 0.49 | 2.1 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 20 | 1.94 | 0.07 | 1.93 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 20 | 1.94 | 0.07 | 1.93 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 20 | 1.94 | 0.07 | 1.93 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 20 | 1.93 | 0.25 | 1.94 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 20 | 1.93 | 0.25 | 1.94 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 20 | 1.93 | 0.25 | 1.94 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 20 | 1.92 | 0.33 | 1.94 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 20 | 1.92 | 0.33 | 1.94 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 20 | 1.91 | 0.43 | 1.9 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 20 | 1.86 | 0.35 | 1.92 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 20 | 1.86 | 0.35 | 1.92 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 20 | 1.86 | 0.35 | 1.92 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 20 | 1.85 | 0.57 | 1.88 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 20 | 1.85 | 0.57 | 1.88 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 20 | 1.85 | 0.57 | 1.88 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 20 | 1.82 | 0.29 | 1.79 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 20 | 1.82 | 0.29 | 1.79 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 20 | 1.82 | 0.29 | 1.79 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 20 | 1.77 | 0.08 | 1.76 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 20 | 1.77 | 0.08 | 1.76 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 20 | 1.77 | 0.08 | 1.76 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 20 | 1.77 | 0.19 | 1.78 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 20 | 1.77 | 0.19 | 1.78 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 20 | 1.77 | 0.19 | 1.78 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 20 | 1.77 | 0.2 | 1.73 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 20 | 1.77 | 0.2 | 1.73 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 20 | 1.77 | 0.2 | 1.73 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 20 | 1.77 | 0.28 | 1.67 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 20 | 1.77 | 0.28 | 1.67 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 20 | 1.77 | 0.28 | 1.67 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 20 | 1.77 | 0.28 | 1.67 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 20 | 1.77 | 0.28 | 1.67 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 20 | 1.77 | 0.28 | 1.67 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 20 | 1.72 | 0.42 | 1.86 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 20 | 1.72 | 0.42 | 1.86 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 20 | 1.72 | 0.42 | 1.86 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 20 | 1.72 | 0.42 | 1.86 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 20 | 1.72 | 0.42 | 1.86 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 20 | 1.72 | 0.42 | 1.86 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 20 | 1.71 | 0.21 | 1.76 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 20 | 1.71 | 0.21 | 1.76 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 20 | 1.71 | 0.21 | 1.76 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 20 | 1.7 | 0.25 | 1.7 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 20 | 1.7 | 0.25 | 1.7 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 20 | 1.7 | 0.25 | 1.7 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 20 | 1.7 | 0.16 | 1.65 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 20 | 1.7 | 0.16 | 1.65 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 20 | 1.7 | 0.16 | 1.65 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 20 | 1.68 | 0.36 | 1.66 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 20 | 1.66 | 0.17 | 1.66 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 20 | 1.66 | 0.17 | 1.66 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 20 | 1.66 | 0.17 | 1.66 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 20 | 1.66 | 0.31 | 1.71 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 20 | 1.66 | 0.31 | 1.71 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 20 | 1.66 | 0.31 | 1.71 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 20 | 1.64 | 0.52 | 1.69 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 20 | 1.64 | 0.52 | 1.69 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 20 | 1.64 | 0.52 | 1.69 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 20 | 1.64 | 0.18 | 1.62 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 20 | 1.63 | 0.18 | 1.64 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 20 | 1.63 | 0.04 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 20 | 1.63 | 0.04 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 20 | 1.63 | 0.04 | 1.65 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 20 | 1.62 | 0.12 | 1.6 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 20 | 1.62 | 0.12 | 1.6 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 20 | 1.62 | 0.12 | 1.6 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 20 | 1.6 | 0.18 | 1.58 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 20 | 1.6 | 0.18 | 1.58 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 20 | 1.6 | 0.18 | 1.58 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 20 | 1.6 | 0.18 | 1.58 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 20 | 1.6 | 0.18 | 1.58 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 20 | 1.6 | 0.18 | 1.58 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 20 | 1.6 | 0.18 | 1.58 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 20 | 1.6 | 0.18 | 1.58 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 20 | 1.6 | 0.18 | 1.58 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 20 | 1.59 | 0.11 | 1.58 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 20 | 1.59 | 0.11 | 1.58 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 20 | 1.59 | 0.11 | 1.58 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 20 | 1.59 | 0.2 | 1.59 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 20 | 1.59 | 0.2 | 1.59 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 20 | 1.59 | 0.2 | 1.59 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 20 | 1.59 | 0.2 | 1.59 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 20 | 1.59 | 0.2 | 1.59 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 20 | 1.59 | 0.2 | 1.59 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 20 | 1.59 | 0.2 | 1.59 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 20 | 1.59 | 0.2 | 1.59 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 20 | 1.59 | 0.2 | 1.59 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 20 | 1.59 | 0.25 | 1.6 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 20 | 1.59 | 0.25 | 1.6 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 20 | 1.59 | 0.25 | 1.6 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 20 | 1.55 | 0.29 | 1.48 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 20 | 1.55 | 0.29 | 1.48 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 20 | 1.55 | 0.29 | 1.48 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 20 | 1.53 | 0.16 | 1.56 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 20 | 1.53 | 0.09 | 1.57 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 20 | 1.53 | 0.09 | 1.57 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 20 | 1.53 | 0.09 | 1.57 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 20 | 1.53 | 0.13 | 1.53 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 20 | 1.53 | 0.13 | 1.53 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 20 | 1.53 | 0.13 | 1.53 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 20 | 1.53 | 0.13 | 1.53 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 20 | 1.53 | 0.13 | 1.53 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 20 | 1.53 | 0.13 | 1.53 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 20 | 1.52 | 0.18 | 1.54 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 20 | 1.52 | 0.18 | 1.54 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 20 | 1.52 | 0.18 | 1.54 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 20 | 1.52 | 0.27 | 1.52 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 20 | 1.52 | 0.27 | 1.52 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 20 | 1.52 | 0.27 | 1.52 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 20 | 1.48 | 0.39 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 20 | 1.48 | 0.39 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 20 | 1.48 | 0.39 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 20 | 1.48 | 0.39 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 20 | 1.48 | 0.39 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 20 | 1.48 | 0.39 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 20 | 1.48 | 0.39 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 20 | 1.48 | 0.39 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 20 | 1.48 | 0.39 | 1.44 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 20 | 1.46 | 0.1 | 1.48 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 20 | 1.46 | 0.1 | 1.48 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 20 | 1.46 | 0.1 | 1.48 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 20 | 1.45 | 0.13 | 1.46 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 20 | 1.45 | 0.13 | 1.46 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 20 | 1.45 | 0.13 | 1.46 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 20 | 1.43 | 0.26 | 1.58 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 20 | 1.43 | 0.26 | 1.58 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 20 | 1.43 | 0.26 | 1.58 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 20 | 1.42 | 0.12 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 20 | 1.42 | 0.12 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 20 | 1.42 | 0.12 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 20 | 1.42 | 0.12 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 20 | 1.42 | 0.12 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 20 | 1.42 | 0.12 | 1.42 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 20 | 1.39 | 0.06 | 1.38 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 20 | 1.39 | 0.06 | 1.38 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 20 | 1.39 | 0.06 | 1.38 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 20 | 1.39 | 0.35 | 1.27 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 20 | 1.39 | 0.35 | 1.27 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 20 | 1.39 | 0.35 | 1.27 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 20 | 1.38 | 0.73 | 1.23 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 20 | 1.38 | 0.73 | 1.23 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 20 | 1.38 | 0.73 | 1.23 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 20 | 1.36 | 0.08 | 1.37 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 20 | 1.36 | 0.08 | 1.37 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 20 | 1.36 | 0.08 | 1.37 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 20 | 1.35 | 0.15 | 1.35 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 20 | 1.35 | 0.35 | 1.35 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 20 | 1.35 | 0.35 | 1.35 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 20 | 1.35 | 0.35 | 1.35 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 20 | 1.35 | 0.27 | 1.34 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 20 | 1.35 | 0.27 | 1.34 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 20 | 1.35 | 0.27 | 1.34 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 20 | 1.33 | 0.08 | 1.37 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 20 | 1.33 | 0.08 | 1.37 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 20 | 1.33 | 0.08 | 1.37 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 20 | 1.33 | 0.27 | 1.27 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 20 | 1.33 | 0.27 | 1.27 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 20 | 1.33 | 0.27 | 1.27 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 20 | 1.31 | 0.24 | 1.38 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 20 | 1.28 | 0.28 | 1.29 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 20 | 1.27 | 0.08 | 1.27 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 20 | 1.27 | 0.08 | 1.27 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 20 | 1.27 | 0.08 | 1.27 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 20 | 1.27 | 0.22 | 1.22 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 20 | 1.27 | 0.22 | 1.22 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 20 | 1.27 | 0.22 | 1.22 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 20 | 1.26 | 0.22 | 1.29 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 20 | 1.26 | 0.11 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 20 | 1.26 | 0.11 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 20 | 1.26 | 0.11 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 20 | 1.26 | 0.11 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 20 | 1.26 | 0.11 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 20 | 1.26 | 0.11 | 1.32 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 20 | 1.26 | 0.19 | 1.23 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 20 | 1.26 | 0.19 | 1.23 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 20 | 1.26 | 0.19 | 1.23 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 20 | 1.24 | 0.14 | 1.24 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 20 | 1.24 | 0.14 | 1.24 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 20 | 1.24 | 0.14 | 1.24 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 20 | 1.24 | 0.14 | 1.24 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 20 | 1.24 | 0.14 | 1.24 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 20 | 1.24 | 0.14 | 1.24 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 20 | 1.24 | 0.14 | 1.24 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 20 | 1.24 | 0.14 | 1.24 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 20 | 1.24 | 0.14 | 1.24 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 20 | 1.23 | 0.28 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 20 | 1.23 | 0.28 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 20 | 1.23 | 0.28 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 20 | 1.23 | 0.28 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 20 | 1.23 | 0.28 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 20 | 1.23 | 0.28 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 20 | 1.23 | 0.28 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 20 | 1.23 | 0.28 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 20 | 1.23 | 0.28 | 1.25 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 20 | 1.23 | 0.2 | 1.27 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 20 | 1.23 | 0.2 | 1.27 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 20 | 1.23 | 0.2 | 1.27 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 20 | 1.22 | 0.18 | 1.18 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 20 | 1.22 | 0.18 | 1.18 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 20 | 1.22 | 0.18 | 1.18 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 20 | 1.22 | 0.29 | 1.23 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 20 | 1.22 | 0.29 | 1.23 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 20 | 1.22 | 0.29 | 1.23 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 20 | 1.21 | 0.49 | 1.28 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 20 | 1.21 | 0.49 | 1.28 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 20 | 1.21 | 0.49 | 1.28 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 20 | 1.21 | 0.49 | 1.28 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 20 | 1.21 | 0.49 | 1.28 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 20 | 1.21 | 0.49 | 1.28 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 20 | 1.21 | 0.49 | 1.28 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 20 | 1.21 | 0.49 | 1.28 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 20 | 1.21 | 0.49 | 1.28 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 20 | 1.2 | 0.28 | 1.25 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 20 | 1.2 | 0.28 | 1.25 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 20 | 1.2 | 0.28 | 1.25 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 20 | 1.19 | 0.32 | 1.23 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 20 | 1.19 | 0.32 | 1.23 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 20 | 1.19 | 0.32 | 1.23 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 20 | 1.18 | 0.17 | 1.16 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 20 | 1.18 | 0.17 | 1.16 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 20 | 1.18 | 0.17 | 1.16 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 20 | 1.17 | 0.24 | 1.04 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 20 | 1.17 | 0.22 | 1.16 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 20 | 1.17 | 0.22 | 1.16 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 20 | 1.17 | 0.22 | 1.16 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 20 | 1.16 | 0.1 | 1.15 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 20 | 1.16 | 0.1 | 1.15 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 20 | 1.16 | 0.1 | 1.15 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 20 | 1.16 | 0.35 | 1.3 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 20 | 1.16 | 0.35 | 1.3 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 20 | 1.16 | 0.35 | 1.3 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 20 | 1.16 | 0.13 | 1.12 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 20 | 1.16 | 0.13 | 1.12 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 20 | 1.16 | 0.13 | 1.12 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 20 | 1.15 | 0.31 | 1.15 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 20 | 1.15 | 0.31 | 1.15 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 20 | 1.15 | 0.31 | 1.15 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 20 | 1.15 | 0.17 | 1.15 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 20 | 1.15 | 0.17 | 1.15 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 20 | 1.15 | 0.17 | 1.15 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 20 | 1.15 | 0.21 | 1.18 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 20 | 1.15 | 0.21 | 1.18 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 20 | 1.15 | 0.21 | 1.18 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 20 | 1.15 | 0.21 | 1.18 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 20 | 1.15 | 0.21 | 1.18 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 20 | 1.15 | 0.21 | 1.18 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 20 | 1.13 | 0.21 | 1.14 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 20 | 1.13 | 0.21 | 1.14 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 20 | 1.13 | 0.21 | 1.14 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 20 | 1.11 | 0.03 | 1.11 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 20 | 1.11 | 0.03 | 1.11 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 20 | 1.11 | 0.03 | 1.11 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 20 | 1.1 | 0.28 | 1.06 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 20 | 1.1 | 0.28 | 1.06 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 20 | 1.1 | 0.28 | 1.06 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 20 | 1.08 | 0.23 | 1.09 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 20 | 1.08 | 0.23 | 1.09 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 20 | 1.08 | 0.23 | 1.09 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 20 | 1.07 | 0.45 | 1.16 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 20 | 1.07 | 0.45 | 1.16 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 20 | 1.07 | 0.45 | 1.16 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 20 | 1.07 | 0.17 | 1.08 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 20 | 1.07 | 0.17 | 1.08 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 20 | 1.07 | 0.17 | 1.08 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 20 | 1.07 | 0.17 | 1.08 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 20 | 1.07 | 0.17 | 1.08 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 20 | 1.07 | 0.17 | 1.08 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 20 | 1.06 | 0.1 | 1.06 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 20 | 1.06 | 0.1 | 1.06 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 20 | 1.06 | 0.1 | 1.06 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 20 | 1.05 | 0.07 | 1.07 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 20 | 1.05 | 0.19 | 1.08 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 20 | 1.05 | 0.19 | 1.08 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 20 | 1.05 | 0.19 | 1.08 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 20 | 1.05 | 0.19 | 1.08 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 20 | 1.05 | 0.19 | 1.08 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 20 | 1.05 | 0.19 | 1.08 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 20 | 1.05 | 0.25 | 0.99 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 20 | 1.05 | 0.25 | 0.99 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 20 | 1.05 | 0.25 | 0.99 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 20 | 1.05 | 0.25 | 0.99 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 20 | 1.05 | 0.25 | 0.99 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 20 | 1.05 | 0.25 | 0.99 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 20 | 1.04 | 0.23 | 1.09 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 20 | 1.02 | 0.25 | 0.94 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 20 | 1.02 | 0.25 | 0.94 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 20 | 1.02 | 0.25 | 0.94 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 20 | 1.02 | 0.21 | 1.0 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 20 | 1.02 | 0.21 | 1.0 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 20 | 1.02 | 0.21 | 1.0 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 20 | 1.02 | 0.16 | 1.03 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 20 | 1.02 | 0.16 | 1.03 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 20 | 1.02 | 0.16 | 1.03 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 20 | 1.02 | 0.29 | 1.16 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 20 | 1.02 | 0.29 | 1.16 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 20 | 1.02 | 0.29 | 1.16 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 20 | 1.01 | 0.16 | 1.0 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 20 | 1.01 | 0.16 | 1.0 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 20 | 1.01 | 0.16 | 1.0 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 20 | 1.0 | 0.1 | 1.01 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 20 | 1.0 | 0.32 | 0.92 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 20 | 1.0 | 0.32 | 0.92 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 20 | 1.0 | 0.32 | 0.92 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 20 | 0.99 | 0.37 | 0.9 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 20 | 0.99 | 0.37 | 0.9 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 20 | 0.99 | 0.13 | 0.99 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 20 | 0.99 | 0.13 | 0.99 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 20 | 0.99 | 0.13 | 0.99 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 20 | 0.97 | 0.1 | 0.94 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 20 | 0.97 | 0.1 | 0.94 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 20 | 0.97 | 0.1 | 0.94 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 20 | 0.96 | 0.13 | 0.97 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 20 | 0.96 | 0.13 | 0.97 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 20 | 0.96 | 0.13 | 0.97 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 20 | 0.96 | 0.27 | 1.04 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 20 | 0.96 | 0.27 | 1.04 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 20 | 0.96 | 0.27 | 1.04 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 20 | 0.95 | 0.14 | 0.98 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 20 | 0.95 | 0.14 | 0.98 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 20 | 0.95 | 0.14 | 0.98 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 20 | 0.95 | 0.2 | 1.01 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 20 | 0.95 | 0.2 | 1.01 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 20 | 0.95 | 0.2 | 1.01 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 20 | 0.95 | 0.33 | 1.02 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 20 | 0.94 | 0.12 | 0.96 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 20 | 0.94 | 0.12 | 0.96 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 20 | 0.94 | 0.12 | 0.96 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 20 | 0.94 | 0.15 | 0.94 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 20 | 0.94 | 0.15 | 0.94 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 20 | 0.94 | 0.15 | 0.94 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 20 | 0.94 | 0.54 | 0.72 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 20 | 0.94 | 0.54 | 0.72 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 20 | 0.94 | 0.54 | 0.72 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 20 | 0.94 | 0.26 | 0.98 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 20 | 0.94 | 0.26 | 0.98 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 20 | 0.93 | 0.25 | 0.99 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 20 | 0.93 | 0.25 | 0.99 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 20 | 0.93 | 0.25 | 0.99 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 20 | 0.92 | 0.18 | 0.94 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 20 | 0.92 | 0.18 | 0.94 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 20 | 0.92 | 0.18 | 0.94 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 20 | 0.92 | 0.07 | 0.92 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 20 | 0.92 | 0.07 | 0.92 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 20 | 0.92 | 0.07 | 0.92 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 20 | 0.91 | 0.08 | 0.92 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 20 | 0.91 | 0.08 | 0.92 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 20 | 0.91 | 0.08 | 0.92 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 20 | 0.91 | 0.16 | 0.94 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 20 | 0.91 | 0.16 | 0.94 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 20 | 0.91 | 0.16 | 0.94 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 20 | 0.91 | 0.09 | 0.92 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 20 | 0.91 | 0.09 | 0.92 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 20 | 0.91 | 0.09 | 0.92 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 20 | 0.91 | 0.09 | 0.92 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 20 | 0.91 | 0.09 | 0.92 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 20 | 0.91 | 0.09 | 0.92 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 20 | 0.91 | 0.21 | 0.93 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 20 | 0.91 | 0.21 | 0.93 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 20 | 0.91 | 0.21 | 0.93 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 20 | 0.9 | 0.59 | 0.7 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 20 | 0.89 | 0.31 | 0.88 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 20 | 0.89 | 0.06 | 0.9 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 20 | 0.89 | 0.06 | 0.9 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 20 | 0.89 | 0.06 | 0.9 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 20 | 0.88 | 0.13 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 20 | 0.88 | 0.13 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 20 | 0.88 | 0.13 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 20 | 0.88 | 0.13 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 20 | 0.88 | 0.13 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 20 | 0.88 | 0.13 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 20 | 0.88 | 0.13 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 20 | 0.88 | 0.13 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 20 | 0.88 | 0.13 | 0.86 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 20 | 0.88 | 0.28 | 0.88 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 20 | 0.88 | 0.28 | 0.88 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 20 | 0.88 | 0.28 | 0.88 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 20 | 0.86 | 0.32 | 0.84 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 20 | 0.86 | 0.32 | 0.84 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 20 | 0.86 | 0.32 | 0.84 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 20 | 0.86 | 0.27 | 0.8 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 20 | 0.86 | 0.27 | 0.8 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 20 | 0.86 | 0.27 | 0.8 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 20 | 0.85 | 0.18 | 0.84 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 20 | 0.85 | 0.18 | 0.84 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 20 | 0.85 | 0.18 | 0.84 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 20 | 0.85 | 0.18 | 0.78 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 20 | 0.84 | 0.22 | 0.86 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 20 | 0.84 | 0.22 | 0.86 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 20 | 0.84 | 0.22 | 0.86 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 20 | 0.83 | 0.3 | 0.87 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 20 | 0.83 | 0.3 | 0.87 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 20 | 0.83 | 0.21 | 0.83 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 20 | 0.82 | 0.2 | 0.9 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 20 | 0.82 | 0.2 | 0.9 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 20 | 0.82 | 0.2 | 0.9 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 20 | 0.82 | 0.02 | 0.83 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 20 | 0.82 | 0.12 | 0.82 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 20 | 0.82 | 0.26 | 0.84 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 20 | 0.82 | 0.26 | 0.84 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 20 | 0.82 | 0.07 | 0.82 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 20 | 0.81 | 0.07 | 0.82 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 20 | 0.81 | 0.07 | 0.82 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 20 | 0.81 | 0.07 | 0.82 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 20 | 0.8 | 0.35 | 0.75 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 20 | 0.79 | 0.16 | 0.78 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 20 | 0.79 | 0.21 | 0.8 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 20 | 0.79 | 0.21 | 0.78 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 20 | 0.77 | 0.27 | 0.72 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 20 | 0.77 | 0.27 | 0.72 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 20 | 0.77 | 0.27 | 0.72 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 20 | 0.77 | 0.24 | 0.95 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 20 | 0.77 | 0.3 | 0.72 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 20 | 0.77 | 0.3 | 0.72 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 20 | 0.77 | 0.3 | 0.72 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 20 | 0.75 | 0.2 | 0.74 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 20 | 0.75 | 0.2 | 0.74 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 20 | 0.75 | 0.29 | 0.82 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 20 | 0.75 | 0.29 | 0.82 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 20 | 0.74 | 0.12 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 20 | 0.74 | 0.12 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 20 | 0.74 | 0.12 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 20 | 0.74 | 0.12 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 20 | 0.74 | 0.12 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 20 | 0.74 | 0.12 | 0.78 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 20 | 0.74 | 0.18 | 0.76 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 20 | 0.74 | 0.18 | 0.76 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 20 | 0.74 | 0.18 | 0.76 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 20 | 0.74 | 0.16 | 0.78 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 20 | 0.74 | 0.16 | 0.78 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 20 | 0.74 | 0.16 | 0.78 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 20 | 0.73 | 0.11 | 0.74 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 20 | 0.73 | 0.11 | 0.74 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 20 | 0.73 | 0.11 | 0.74 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 20 | 0.72 | 0.11 | 0.76 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 20 | 0.72 | 0.27 | 0.73 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 20 | 0.72 | 0.27 | 0.73 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 20 | 0.72 | 0.27 | 0.73 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 20 | 0.72 | 0.27 | 0.73 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 20 | 0.71 | 0.23 | 0.74 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 20 | 0.7 | 0.17 | 0.68 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 20 | 0.7 | 0.17 | 0.68 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 20 | 0.7 | 0.17 | 0.68 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 20 | 0.68 | 0.12 | 0.68 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 20 | 0.68 | 0.12 | 0.68 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 20 | 0.68 | 0.12 | 0.68 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 20 | 0.68 | 0.12 | 0.68 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 20 | 0.68 | 0.12 | 0.68 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 20 | 0.68 | 0.12 | 0.68 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 20 | 0.68 | 0.09 | 0.66 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 20 | 0.68 | 0.09 | 0.66 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 20 | 0.68 | 0.09 | 0.66 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 20 | 0.67 | 0.28 | 0.62 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 20 | 0.67 | 0.28 | 0.62 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 20 | 0.67 | 0.28 | 0.62 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 20 | 0.67 | 0.09 | 0.68 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 20 | 0.66 | 0.21 | 0.64 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 20 | 0.66 | 0.21 | 0.64 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 20 | 0.66 | 0.21 | 0.64 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 20 | 0.66 | 0.09 | 0.68 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 20 | 0.66 | 0.09 | 0.68 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 20 | 0.66 | 0.09 | 0.68 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 20 | 0.65 | 0.12 | 0.67 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 20 | 0.65 | 0.28 | 0.75 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 20 | 0.63 | 0.1 | 0.62 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 20 | 0.63 | 0.1 | 0.62 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 20 | 0.63 | 0.1 | 0.62 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 20 | 0.63 | 0.2 | 0.63 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 20 | 0.63 | 0.2 | 0.63 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 20 | 0.63 | 0.2 | 0.63 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 20 | 0.62 | 0.07 | 0.62 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 20 | 0.62 | 0.04 | 0.62 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 20 | 0.61 | 0.18 | 0.53 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 20 | 0.61 | 0.18 | 0.53 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 20 | 0.61 | 0.18 | 0.53 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 20 | 0.6 | 0.21 | 0.5 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 20 | 0.6 | 0.21 | 0.5 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 20 | 0.6 | 0.21 | 0.5 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 20 | 0.6 | 0.05 | 0.62 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 20 | 0.6 | 0.05 | 0.62 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 20 | 0.6 | 0.05 | 0.62 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 20 | 0.6 | 0.08 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 20 | 0.6 | 0.08 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 20 | 0.6 | 0.08 | 0.61 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 20 | 0.6 | 0.18 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 20 | 0.6 | 0.18 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 20 | 0.6 | 0.18 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 20 | 0.6 | 0.18 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 20 | 0.6 | 0.18 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 20 | 0.6 | 0.18 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 20 | 0.6 | 0.18 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 20 | 0.6 | 0.18 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 20 | 0.6 | 0.18 | 0.58 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 20 | 0.59 | 0.2 | 0.56 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 20 | 0.59 | 0.2 | 0.56 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 20 | 0.59 | 0.2 | 0.56 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 20 | 0.59 | 0.2 | 0.56 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 20 | 0.59 | 0.2 | 0.56 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 20 | 0.59 | 0.2 | 0.56 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 20 | 0.59 | 0.08 | 0.57 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 20 | 0.58 | 0.19 | 0.6 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 20 | 0.58 | 0.19 | 0.6 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 20 | 0.58 | 0.19 | 0.6 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 20 | 0.58 | 0.19 | 0.6 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 20 | 0.58 | 0.19 | 0.6 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 20 | 0.58 | 0.19 | 0.6 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 20 | 0.58 | 0.17 | 0.6 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 20 | 0.58 | 0.02 | 0.58 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 20 | 0.58 | 0.02 | 0.58 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 20 | 0.58 | 0.02 | 0.58 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 20 | 0.57 | 0.13 | 0.56 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 20 | 0.57 | 0.13 | 0.56 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 20 | 0.57 | 0.13 | 0.56 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 20 | 0.56 | 0.05 | 0.57 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 20 | 0.56 | 0.05 | 0.57 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 20 | 0.56 | 0.05 | 0.57 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 20 | 0.56 | 0.29 | 0.57 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 20 | 0.56 | 0.29 | 0.57 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 20 | 0.56 | 0.29 | 0.57 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 20 | 0.56 | 0.29 | 0.57 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 20 | 0.56 | 0.29 | 0.57 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 20 | 0.56 | 0.29 | 0.57 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 20 | 0.56 | 0.29 | 0.57 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 20 | 0.56 | 0.29 | 0.57 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 20 | 0.56 | 0.29 | 0.57 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 20 | 0.56 | 0.08 | 0.56 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 20 | 0.56 | 0.04 | 0.56 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 20 | 0.56 | 0.04 | 0.56 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 20 | 0.56 | 0.04 | 0.56 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 20 | 0.56 | 0.04 | 0.56 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 20 | 0.55 | 0.23 | 0.52 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 20 | 0.55 | 0.23 | 0.52 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 20 | 0.55 | 0.23 | 0.52 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 20 | 0.54 | 0.17 | 0.55 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 20 | 0.54 | 0.17 | 0.55 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 20 | 0.54 | 0.17 | 0.55 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 20 | 0.53 | 0.16 | 0.54 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 20 | 0.53 | 0.16 | 0.54 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 20 | 0.53 | 0.16 | 0.54 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 20 | 0.53 | 0.16 | 0.54 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 20 | 0.53 | 0.16 | 0.54 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 20 | 0.53 | 0.16 | 0.54 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 20 | 0.53 | 0.03 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 20 | 0.53 | 0.03 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 20 | 0.53 | 0.03 | 0.53 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 20 | 0.53 | 0.12 | 0.5 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 20 | 0.53 | 0.16 | 0.49 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 20 | 0.53 | 0.16 | 0.49 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 20 | 0.52 | 0.03 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 20 | 0.52 | 0.03 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 20 | 0.52 | 0.03 | 0.53 |
| (1,441) | 1:34:A:TYR:HE2 | 1:92:A:PHE:H | 20 | 0.52 | 0.24 | 0.59 |
| (1,441) | 1:34:A:TYR:HE1 | 1:92:A:PHE:H | 20 | 0.52 | 0.24 | 0.59 |
| (1,441) | 1:34:A:TYR:HD2 | 1:92:A:PHE:H | 20 | 0.52 | 0.24 | 0.59 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 20 | 0.51 | 0.21 | 0.56 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 20 | 0.51 | 0.21 | 0.56 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 20 | 0.51 | 0.21 | 0.56 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 20 | 0.51 | 0.04 | 0.52 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 20 | 0.51 | 0.04 | 0.52 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 20 | 0.51 | 0.16 | 0.52 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 20 | 0.51 | 0.16 | 0.52 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 20 | 0.51 | 0.16 | 0.52 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 20 | 0.5 | 0.08 | 0.5 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 20 | 0.49 | 0.2 | 0.46 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 20 | 0.49 | 0.02 | 0.49 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 20 | 0.49 | 0.02 | 0.49 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 20 | 0.49 | 0.02 | 0.49 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 20 | 0.49 | 0.03 | 0.48 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 20 | 0.49 | 0.03 | 0.48 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 20 | 0.49 | 0.03 | 0.48 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 20 | 0.49 | 0.07 | 0.5 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 20 | 0.49 | 0.07 | 0.5 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 20 | 0.49 | 0.07 | 0.5 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 20 | 0.46 | 0.17 | 0.48 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 20 | 0.46 | 0.12 | 0.47 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 20 | 0.46 | 0.12 | 0.47 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 20 | 0.46 | 0.12 | 0.47 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 20 | 0.45 | 0.1 | 0.43 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 20 | 0.45 | 0.1 | 0.43 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 20 | 0.45 | 0.1 | 0.43 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 20 | 0.44 | 0.16 | 0.43 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 20 | 0.44 | 0.16 | 0.43 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 20 | 0.44 | 0.16 | 0.43 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 20 | 0.44 | 0.13 | 0.44 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 20 | 0.42 | 0.08 | 0.44 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 20 | 0.41 | 0.05 | 0.42 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 20 | 0.41 | 0.02 | 0.41 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 20 | 0.41 | 0.02 | 0.41 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 20 | 0.41 | 0.02 | 0.41 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 20 | 0.39 | 0.06 | 0.4 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 20 | 0.39 | 0.03 | 0.38 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 20 | 0.39 | 0.03 | 0.38 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 20 | 0.39 | 0.03 | 0.38 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 20 | 0.37 | 0.07 | 0.38 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 20 | 0.37 | 0.1 | 0.37 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 20 | 0.37 | 0.1 | 0.37 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 20 | 0.37 | 0.1 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 20 | 0.36 | 0.1 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 20 | 0.36 | 0.1 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 20 | 0.36 | 0.1 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 20 | 0.36 | 0.1 | 0.37 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 20 | 0.36 | 0.1 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 20 | 0.36 | 0.1 | 0.37 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 20 | 0.34 | 0.02 | 0.34 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 20 | 0.34 | 0.02 | 0.34 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 20 | 0.34 | 0.02 | 0.34 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 20 | 0.34 | 0.03 | 0.34 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 20 | 0.34 | 0.03 | 0.34 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 20 | 0.34 | 0.03 | 0.34 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 20 | 0.34 | 0.08 | 0.32 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 20 | 0.34 | 0.09 | 0.34 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 20 | 0.34 | 0.09 | 0.34 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 20 | 0.34 | 0.09 | 0.34 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 20 | 0.34 | 0.07 | 0.36 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 20 | 0.34 | 0.05 | 0.34 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 20 | 0.32 | 0.09 | 0.33 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 20 | 0.31 | 0.02 | 0.32 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 20 | 0.3 | 0.11 | 0.28 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 20 | 0.3 | 0.1 | 0.28 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 20 | 0.3 | 0.01 | 0.3 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 20 | 0.27 | 0.07 | 0.26 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 20 | 0.26 | 0.07 | 0.25 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 20 | 0.26 | 0.07 | 0.25 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 20 | 0.26 | 0.07 | 0.25 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 20 | 0.25 | 0.06 | 0.25 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 20 | 0.25 | 0.06 | 0.25 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 20 | 0.25 | 0.06 | 0.25 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 20 | 0.23 | 0.02 | 0.23 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 20 | 0.23 | 0.02 | 0.23 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 20 | 0.23 | 0.02 | 0.23 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 20 | 0.23 | 0.02 | 0.23 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 20 | 0.21 | 0.04 | 0.2 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 20 | 0.15 | 0.01 | 0.15 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 19 | 2.0 | 0.23 | 2.0 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 19 | 2.0 | 0.23 | 2.0 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 19 | 2.0 | 0.23 | 2.0 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 19 | 1.63 | 0.9 | 1.5 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 19 | 1.63 | 0.9 | 1.5 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 19 | 1.63 | 0.9 | 1.5 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 19 | 1.36 | 0.36 | 1.31 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 19 | 1.36 | 0.36 | 1.31 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 19 | 1.2 | 0.8 | 0.84 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 19 | 1.2 | 0.8 | 0.84 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 19 | 1.12 | 0.44 | 1.18 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 19 | 1.12 | 0.44 | 1.18 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 19 | 1.12 | 0.44 | 1.18 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 19 | 0.98 | 0.3 | 1.05 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 19 | 0.95 | 0.22 | 0.98 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 19 | 0.89 | 0.18 | 0.91 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 19 | 0.89 | 0.18 | 0.91 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 19 | 0.89 | 0.18 | 0.91 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 19 | 0.85 | 0.36 | 0.95 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 19 | 0.85 | 0.36 | 0.95 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 19 | 0.85 | 0.36 | 0.95 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 19 | 0.8 | 0.3 | 0.86 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 19 | 0.73 | 0.09 | 0.72 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 19 | 0.72 | 0.13 | 0.68 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 19 | 0.71 | 0.36 | 0.75 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 19 | 0.71 | 0.36 | 0.75 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 19 | 0.71 | 0.36 | 0.75 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 19 | 0.67 | 0.31 | 0.64 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 19 | 0.67 | 0.44 | 0.44 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 19 | 0.67 | 0.44 | 0.44 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 19 | 0.67 | 0.44 | 0.44 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 19 | 0.62 | 0.16 | 0.66 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 19 | 0.56 | 0.33 | 0.62 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 19 | 0.55 | 0.2 | 0.6 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 19 | 0.55 | 0.2 | 0.6 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 19 | 0.55 | 0.2 | 0.6 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 19 | 0.55 | 0.2 | 0.6 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 19 | 0.55 | 0.2 | 0.6 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 19 | 0.55 | 0.2 | 0.6 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 19 | 0.54 | 0.11 | 0.58 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 19 | 0.53 | 0.18 | 0.48 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 19 | 0.53 | 0.18 | 0.48 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 19 | 0.53 | 0.18 | 0.48 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 19 | 0.51 | 0.25 | 0.42 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 19 | 0.51 | 0.25 | 0.42 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 19 | 0.51 | 0.25 | 0.42 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 19 | 0.51 | 0.25 | 0.42 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 19 | 0.51 | 0.25 | 0.42 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 19 | 0.51 | 0.25 | 0.42 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 19 | 0.5 | 0.04 | 0.52 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 19 | 0.49 | 0.17 | 0.55 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 19 | 0.49 | 0.17 | 0.55 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 19 | 0.47 | 0.12 | 0.5 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 19 | 0.47 | 0.12 | 0.5 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 19 | 0.47 | 0.12 | 0.5 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 19 | 0.47 | 0.13 | 0.54 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 19 | 0.42 | 0.19 | 0.46 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 19 | 0.42 | 0.19 | 0.46 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 19 | 0.42 | 0.19 | 0.46 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 19 | 0.42 | 0.14 | 0.46 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 19 | 0.42 | 0.19 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 19 | 0.42 | 0.19 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 19 | 0.42 | 0.19 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 19 | 0.42 | 0.19 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 19 | 0.42 | 0.19 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 19 | 0.42 | 0.19 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 19 | 0.42 | 0.19 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 19 | 0.42 | 0.19 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 19 | 0.42 | 0.19 | 0.4 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 19 | 0.38 | 0.19 | 0.33 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 19 | 0.38 | 0.19 | 0.33 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 19 | 0.38 | 0.19 | 0.33 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 19 | 0.38 | 0.08 | 0.39 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 19 | 0.37 | 0.16 | 0.31 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 19 | 0.36 | 0.06 | 0.36 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 19 | 0.35 | 0.09 | 0.37 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 19 | 0.35 | 0.09 | 0.37 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 19 | 0.35 | 0.09 | 0.37 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 19 | 0.34 | 0.19 | 0.3 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 19 | 0.33 | 0.1 | 0.33 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 19 | 0.32 | 0.14 | 0.3 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 19 | 0.3 | 0.07 | 0.29 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 19 | 0.3 | 0.13 | 0.25 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 19 | 0.3 | 0.1 | 0.29 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 19 | 0.29 | 0.06 | 0.3 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 19 | 0.28 | 0.03 | 0.29 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 19 | 0.28 | 0.05 | 0.28 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 19 | 0.28 | 0.1 | 0.28 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 19 | 0.28 | 0.1 | 0.28 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 19 | 0.28 | 0.1 | 0.28 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 19 | 0.27 | 0.1 | 0.28 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 19 | 0.27 | 0.04 | 0.28 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 19 | 0.24 | 0.06 | 0.26 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 19 | 0.24 | 0.06 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 19 | 0.24 | 0.06 | 0.26 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 19 | 0.24 | 0.06 | 0.26 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 19 | 0.24 | 0.06 | 0.26 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 19 | 0.24 | 0.06 | 0.26 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 19 | 0.24 | 0.06 | 0.26 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 19 | 0.24 | 0.06 | 0.26 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 19 | 0.24 | 0.06 | 0.26 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 19 | 0.24 | 0.09 | 0.22 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 19 | 0.22 | 0.1 | 0.22 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 19 | 0.14 | 0.01 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 19 | 0.14 | 0.01 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 19 | 0.14 | 0.01 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 19 | 0.14 | 0.01 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 19 | 0.14 | 0.01 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 19 | 0.14 | 0.01 | 0.14 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 19 | 0.14 | 0.01 | 0.14 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 19 | 0.12 | 0.01 | 0.12 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 19 | 0.12 | 0.01 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 19 | 0.11 | 0.01 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 19 | 0.11 | 0.01 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 19 | 0.11 | 0.01 | 0.11 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 18 | 2.67 | 1.12 | 2.75 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 18 | 2.67 | 1.12 | 2.75 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 18 | 2.67 | 1.12 | 2.75 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 18 | 1.59 | 0.61 | 1.8 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 18 | 1.59 | 0.61 | 1.8 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 18 | 1.59 | 0.61 | 1.8 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 18 | 1.59 | 0.61 | 1.8 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 18 | 1.59 | 0.61 | 1.8 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 18 | 1.59 | 0.61 | 1.8 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 18 | 1.11 | 0.35 | 1.12 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 18 | 1.0 | 0.36 | 1.08 |
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 18 | 0.96 | 0.5 | 1.0 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 18 | 0.84 | 0.36 | 0.91 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 18 | 0.84 | 0.36 | 0.91 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 18 | 0.84 | 0.36 | 0.91 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 18 | 0.84 | 0.56 | 0.51 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 18 | 0.84 | 0.56 | 0.51 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 18 | 0.84 | 0.56 | 0.51 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 18 | 0.79 | 0.17 | 0.78 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 18 | 0.76 | 0.26 | 0.72 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 18 | 0.68 | 0.04 | 0.69 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 18 | 0.68 | 0.21 | 0.72 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 18 | 0.51 | 0.3 | 0.51 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 18 | 0.51 | 0.3 | 0.51 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 18 | 0.51 | 0.3 | 0.51 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 18 | 0.5 | 0.21 | 0.48 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 18 | 0.46 | 0.26 | 0.31 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 18 | 0.45 | 0.19 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 18 | 0.45 | 0.19 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 18 | 0.45 | 0.19 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 18 | 0.45 | 0.19 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 18 | 0.45 | 0.19 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 18 | 0.45 | 0.19 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 18 | 0.45 | 0.19 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 18 | 0.45 | 0.19 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 18 | 0.45 | 0.19 | 0.42 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 18 | 0.29 | 0.1 | 0.3 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 18 | 0.29 | 0.1 | 0.3 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 18 | 0.29 | 0.1 | 0.3 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 18 | 0.29 | 0.1 | 0.3 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 18 | 0.29 | 0.1 | 0.3 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 18 | 0.29 | 0.1 | 0.3 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 18 | 0.28 | 0.09 | 0.28 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 18 | 0.27 | 0.06 | 0.26 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 18 | 0.27 | 0.06 | 0.26 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 18 | 0.27 | 0.06 | 0.26 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 18 | 0.27 | 0.06 | 0.26 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 18 | 0.27 | 0.06 | 0.26 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 18 | 0.27 | 0.06 | 0.26 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 18 | 0.26 | 0.07 | 0.27 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 18 | 0.26 | 0.07 | 0.27 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 18 | 0.26 | 0.07 | 0.27 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 18 | 0.23 | 0.21 | 0.13 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 18 | 0.23 | 0.06 | 0.22 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 18 | 0.23 | 0.06 | 0.22 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 18 | 0.23 | 0.06 | 0.22 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 18 | 0.19 | 0.06 | 0.18 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 18 | 0.13 | 0.01 | 0.13 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 18 | 0.11 | 0.0 | 0.11 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 17 | 1.21 | 0.51 | 1.34 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 17 | 1.21 | 0.51 | 1.34 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 17 | 1.21 | 0.51 | 1.34 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 17 | 1.2 | 0.47 | 1.21 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 17 | 1.2 | 0.47 | 1.21 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 17 | 1.2 | 0.47 | 1.21 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 17 | 1.2 | 0.47 | 1.21 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 17 | 1.2 | 0.47 | 1.21 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 17 | 1.2 | 0.47 | 1.21 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 17 | 1.2 | 0.47 | 1.21 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 17 | 1.2 | 0.47 | 1.21 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 17 | 1.2 | 0.47 | 1.21 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 17 | 0.97 | 0.59 | 0.9 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 17 | 0.97 | 0.59 | 0.9 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 17 | 0.97 | 0.59 | 0.9 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 17 | 0.81 | 0.38 | 0.78 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 17 | 0.81 | 0.38 | 0.78 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 17 | 0.75 | 0.2 | 0.78 |
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 17 | 0.67 | 0.19 | 0.68 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 17 | 0.67 | 0.19 | 0.68 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 17 | 0.67 | 0.19 | 0.68 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 17 | 0.52 | 0.27 | 0.45 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 17 | 0.52 | 0.27 | 0.45 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 17 | 0.52 | 0.27 | 0.45 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 17 | 0.5 | 0.23 | 0.45 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 17 | 0.49 | 0.25 | 0.37 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 17 | 0.49 | 0.25 | 0.37 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 17 | 0.49 | 0.25 | 0.37 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 17 | 0.44 | 0.16 | 0.44 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 17 | 0.39 | 0.18 | 0.34 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 17 | 0.39 | 0.18 | 0.34 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 17 | 0.35 | 0.16 | 0.39 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 17 | 0.35 | 0.16 | 0.39 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 17 | 0.32 | 0.15 | 0.3 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 17 | 0.31 | 0.16 | 0.29 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 17 | 0.31 | 0.16 | 0.29 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 17 | 0.31 | 0.16 | 0.29 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 17 | 0.31 | 0.16 | 0.29 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 17 | 0.31 | 0.16 | 0.29 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 17 | 0.31 | 0.16 | 0.29 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 17 | 0.31 | 0.08 | 0.34 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 17 | 0.31 | 0.08 | 0.34 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 17 | 0.31 | 0.08 | 0.34 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 17 | 0.3 | 0.05 | 0.3 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 17 | 0.26 | 0.08 | 0.25 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 17 | 0.26 | 0.08 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 17 | 0.26 | 0.08 | 0.25 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 17 | 0.24 | 0.1 | 0.22 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 17 | 0.24 | 0.1 | 0.22 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 17 | 0.24 | 0.1 | 0.22 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 17 | 0.23 | 0.06 | 0.23 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 17 | 0.19 | 0.04 | 0.21 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 17 | 0.19 | 0.04 | 0.21 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 17 | 0.19 | 0.04 | 0.21 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 17 | 0.19 | 0.08 | 0.17 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 17 | 0.14 | 0.01 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 17 | 0.14 | 0.01 | 0.14 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 17 | 0.11 | 0.01 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 17 | 0.11 | 0.01 | 0.11 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 16 | 1.76 | 0.3 | 1.72 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 16 | 1.44 | 0.63 | 1.4 |
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 16 | 1.24 | 0.23 | 1.26 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 16 | 1.24 | 0.23 | 1.26 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 16 | 1.14 | 0.24 | 1.13 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 16 | 1.13 | 0.36 | 1.27 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 16 | 1.03 | 0.33 | 0.97 |
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 16 | 0.96 | 0.08 | 0.96 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 16 | 0.89 | 0.31 | 0.86 |
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 16 | 0.82 | 0.13 | 0.84 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 16 | 0.81 | 0.22 | 0.8 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 16 | 0.78 | 0.1 | 0.78 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 16 | 0.72 | 0.25 | 0.76 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 16 | 0.71 | 0.13 | 0.75 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 16 | 0.67 | 0.1 | 0.7 |
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 16 | 0.64 | 0.03 | 0.64 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 16 | 0.63 | 0.16 | 0.62 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 16 | 0.58 | 0.33 | 0.53 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 16 | 0.58 | 0.33 | 0.53 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 16 | 0.58 | 0.33 | 0.53 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 16 | 0.58 | 0.33 | 0.53 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 16 | 0.58 | 0.33 | 0.53 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 16 | 0.58 | 0.33 | 0.53 |
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 16 | 0.56 | 0.3 | 0.61 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 16 | 0.52 | 0.33 | 0.44 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 16 | 0.52 | 0.33 | 0.44 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 16 | 0.52 | 0.33 | 0.44 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 16 | 0.52 | 0.33 | 0.44 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 16 | 0.52 | 0.33 | 0.44 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 16 | 0.52 | 0.33 | 0.44 |
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 16 | 0.49 | 0.16 | 0.56 |
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 16 | 0.49 | 0.16 | 0.56 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 16 | 0.47 | 0.24 | 0.36 |
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 16 | 0.43 | 0.07 | 0.42 |
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 16 | 0.43 | 0.2 | 0.47 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 16 | 0.42 | 0.17 | 0.44 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 16 | 0.42 | 0.17 | 0.44 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 16 | 0.37 | 0.18 | 0.35 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 16 | 0.37 | 0.18 | 0.35 |
| (1,1080) | 1:34:A:TYR:HD1 | 1:38:A:GLU:H | 16 | 0.37 | 0.2 | 0.32 |
| (1,1080) | 1:34:A:TYR:HD2 | 1:38:A:GLU:H | 16 | 0.37 | 0.2 | 0.32 |
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 16 | 0.36 | 0.13 | 0.34 |
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 16 | 0.36 | 0.13 | 0.34 |
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 16 | 0.36 | 0.13 | 0.36 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 16 | 0.36 | 0.13 | 0.36 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 16 | 0.36 | 0.13 | 0.36 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 16 | 0.35 | 0.08 | 0.35 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 16 | 0.34 | 0.15 | 0.34 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 16 | 0.33 | 0.08 | 0.37 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 16 | 0.32 | 0.12 | 0.3 |
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 16 | 0.31 | 0.14 | 0.33 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 16 | 0.3 | 0.07 | 0.3 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 16 | 0.3 | 0.07 | 0.3 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 16 | 0.3 | 0.07 | 0.3 |
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 16 | 0.29 | 0.05 | 0.32 |
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 16 | 0.28 | 0.13 | 0.22 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 16 | 0.28 | 0.06 | 0.27 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 16 | 0.27 | 0.06 | 0.29 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 16 | 0.26 | 0.11 | 0.26 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 16 | 0.25 | 0.07 | 0.23 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 16 | 0.25 | 0.07 | 0.23 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 16 | 0.25 | 0.07 | 0.23 |
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 16 | 0.25 | 0.12 | 0.2 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 16 | 0.23 | 0.07 | 0.24 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 16 | 0.23 | 0.07 | 0.24 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 16 | 0.23 | 0.07 | 0.24 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 16 | 0.23 | 0.07 | 0.24 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 16 | 0.23 | 0.07 | 0.24 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 16 | 0.23 | 0.07 | 0.24 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 16 | 0.23 | 0.07 | 0.24 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 16 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 16 | 0.23 | 0.07 | 0.24 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 16 | 0.16 | 0.03 | 0.16 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 16 | 0.14 | 0.01 | 0.15 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 16 | 0.12 | 0.01 | 0.11 |
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 16 | 0.11 | 0.0 | 0.11 |
| (1,1578) | 1:118:A:GLY:H | 1:119:A:GLU:HG3 | 15 | 1.13 | 0.3 | 1.19 |
| (1,112) | 1:105:A:ALA:H | 1:106:A:ASP:HB3 | 15 | 0.96 | 0.15 | 1.0 |
| (1,2015) | 1:117:A:LYS:HB2 | 1:117:A:LYS:HD3 | 15 | 0.85 | 0.4 | 1.04 |
| (1,3480) | 1:32:A:HIS:HD2 | 1:150:A:PRO:HG3 | 15 | 0.81 | 0.47 | 0.97 |
| (1,353) | 1:108:A:ARG:HG3 | 1:112:A:VAL:H | 15 | 0.77 | 0.43 | 0.96 |
| (1,163) | 1:69:A:LYS:H | 1:70:A:ASP:HB3 | 15 | 0.76 | 0.16 | 0.78 |
| (1,1058) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HA | 15 | 0.75 | 0.32 | 0.85 |
| (1,894) | 1:103:A:SER:H | 1:106:A:ASP:HB3 | 15 | 0.69 | 0.1 | 0.68 |
| (1,90) | 1:185:A:VAL:HA | 1:188:A:LYS:H | 15 | 0.67 | 0.27 | 0.72 |
| (1,1409) | 1:67:A:LEU:HB2 | 1:70:A:ASP:HB3 | 15 | 0.66 | 0.21 | 0.6 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB2 | 15 | 0.64 | 0.31 | 0.58 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB3 | 15 | 0.64 | 0.31 | 0.58 |
| (1,683) | 1:168:A:SER:H | 1:170:A:MET:HG2 | 15 | 0.62 | 0.25 | 0.68 |
| (1,991) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HD22 | 15 | 0.58 | 0.25 | 0.53 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG21 | 15 | 0.57 | 0.12 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG22 | 15 | 0.57 | 0.12 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG23 | 15 | 0.57 | 0.12 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG21 | 15 | 0.57 | 0.12 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG22 | 15 | 0.57 | 0.12 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG23 | 15 | 0.57 | 0.12 | 0.54 |
| (1,883) | 1:49:A:LYS:H | 1:49:A:LYS:HD3 | 15 | 0.49 | 0.25 | 0.51 |
| (1,765) | 1:106:A:ASP:H | 1:106:A:ASP:HB3 | 15 | 0.47 | 0.05 | 0.46 |
| (1,778) | 1:51:A:PRO:HB3 | 1:54:A:THR:H | 15 | 0.46 | 0.42 | 0.32 |
| (1,1191) | 1:64:A:LEU:HD11 | 1:65:A:GLY:H | 15 | 0.45 | 0.12 | 0.49 |
| (1,1191) | 1:64:A:LEU:HD12 | 1:65:A:GLY:H | 15 | 0.45 | 0.12 | 0.49 |
| (1,1191) | 1:64:A:LEU:HD13 | 1:65:A:GLY:H | 15 | 0.45 | 0.12 | 0.49 |
| (1,2452) | 1:149:A:VAL:HG11 | 1:150:A:PRO:HG3 | 15 | 0.44 | 0.14 | 0.48 |
| (1,2452) | 1:149:A:VAL:HG12 | 1:150:A:PRO:HG3 | 15 | 0.44 | 0.14 | 0.48 |
| (1,2452) | 1:149:A:VAL:HG13 | 1:150:A:PRO:HG3 | 15 | 0.44 | 0.14 | 0.48 |
| (1,2452) | 1:149:A:VAL:HG21 | 1:150:A:PRO:HG3 | 15 | 0.44 | 0.14 | 0.48 |
| (1,2452) | 1:149:A:VAL:HG22 | 1:150:A:PRO:HG3 | 15 | 0.44 | 0.14 | 0.48 |
| (1,2452) | 1:149:A:VAL:HG23 | 1:150:A:PRO:HG3 | 15 | 0.44 | 0.14 | 0.48 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG11 | 15 | 0.44 | 0.28 | 0.4 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG12 | 15 | 0.44 | 0.28 | 0.4 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG13 | 15 | 0.44 | 0.28 | 0.4 |
| (1,3269) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA2 | 15 | 0.44 | 0.23 | 0.39 |
| (1,3269) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA2 | 15 | 0.44 | 0.23 | 0.39 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3269) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA2 | 15 | 0.44 | 0.23 | 0.39 |
| (1,127) | 1:105:A:ALA:H | 1:107:A:ILE:HB | 15 | 0.43 | 0.14 | 0.4 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG11 | 15 | 0.43 | 0.23 | 0.34 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG12 | 15 | 0.43 | 0.23 | 0.34 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG13 | 15 | 0.43 | 0.23 | 0.34 |
| (1,3311) | 1:29:A:TYR:HD1 | 1:71:A:LEU:HB2 | 15 | 0.42 | 0.17 | 0.43 |
| (1,3311) | 1:29:A:TYR:HD2 | 1:71:A:LEU:HB2 | 15 | 0.42 | 0.17 | 0.43 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE2 | 15 | 0.42 | 0.18 | 0.47 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE3 | 15 | 0.42 | 0.18 | 0.47 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE2 | 15 | 0.42 | 0.18 | 0.47 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE3 | 15 | 0.42 | 0.18 | 0.47 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE2 | 15 | 0.42 | 0.18 | 0.47 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE3 | 15 | 0.42 | 0.18 | 0.47 |
| (1,1164) | 1:27:A:SER:H | 1:30:A:CYS:HB3 | 15 | 0.31 | 0.11 | 0.33 |
| (1,1005) | 1:46:A:VAL:HG21 | 1:48:A:GLN:H | 15 | 0.27 | 0.07 | 0.27 |
| (1,1005) | 1:46:A:VAL:HG22 | 1:48:A:GLN:H | 15 | 0.27 | 0.07 | 0.27 |
| (1,1005) | 1:46:A:VAL:HG23 | 1:48:A:GLN:H | 15 | 0.27 | 0.07 | 0.27 |
| (1,1565) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 15 | 0.26 | 0.09 | 0.25 |
| (1,1695) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HE22 | 15 | 0.25 | 0.08 | 0.28 |
| (1,1438) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HB2 | 15 | 0.23 | 0.1 | 0.19 |
| (1,1438) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HB2 | 15 | 0.23 | 0.1 | 0.19 |
| (1,1438) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HB2 | 15 | 0.23 | 0.1 | 0.19 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG11 | 15 | 0.21 | 0.08 | 0.22 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG12 | 15 | 0.21 | 0.08 | 0.22 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG13 | 15 | 0.21 | 0.08 | 0.22 |
| (1,967) | 1:126:A:ASN:HB2 | 1:126:A:ASN:HD22 | 15 | 0.2 | 0.02 | 0.21 |
| (1,2315) | 1:46:A:VAL:HG21 | 1:50:A:LEU:HG | 15 | 0.2 | 0.12 | 0.17 |
| (1,2315) | 1:46:A:VAL:HG22 | 1:50:A:LEU:HG | 15 | 0.2 | 0.12 | 0.17 |
| (1,2315) | 1:46:A:VAL:HG23 | 1:50:A:LEU:HG | 15 | 0.2 | 0.12 | 0.17 |
| (1,2753) | 1:61:A:VAL:HG11 | 1:62:A:GLU:HA | 15 | 0.18 | 0.05 | 0.2 |
| (1,2753) | 1:61:A:VAL:HG12 | 1:62:A:GLU:HA | 15 | 0.18 | 0.05 | 0.2 |
| (1,2753) | 1:61:A:VAL:HG13 | 1:62:A:GLU:HA | 15 | 0.18 | 0.05 | 0.2 |
| (1,568) | 1:49:A:LYS:HA | 1:50:A:LEU:H | 15 | 0.17 | 0.03 | 0.17 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG21 | 15 | 0.15 | 0.02 | 0.14 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG22 | 15 | 0.15 | 0.02 | 0.14 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG23 | 15 | 0.15 | 0.02 | 0.14 |
| (1,138) | 1:80:A:ALA:H | 1:81:A:LEU:HA | 15 | 0.13 | 0.02 | 0.14 |
| (1,1351) | 1:179:A:ASP:HB2 | 1:183:A:GLN:HE21 | 14 | 1.5 | 0.56 | 1.71 |
| (1,102) | 1:50:A:LEU:HD21 | 1:56:A:MET:H | 14 | 0.88 | 0.35 | 0.82 |
| (1,102) | 1:50:A:LEU:HD22 | 1:56:A:MET:H | 14 | 0.88 | 0.35 | 0.82 |
| (1,102) | 1:50:A:LEU:HD23 | 1:56:A:MET:H | 14 | 0.88 | 0.35 | 0.82 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG12 | 14 | 0.69 | 0.25 | 0.72 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG13 | 14 | 0.69 | 0.25 | 0.72 |
| (1,1581) | 1:62:A:GLU:HA | 1:62:A:GLU:HG2 | 14 | 0.45 | 0.04 | 0.46 |
| (1,1588) | 1:62:A:GLU:HA | 1:62:A:GLU:HG3 | 14 | 0.43 | 0.07 | 0.46 |
| (1,2168) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HG2 | 14 | 0.42 | 0.23 | 0.44 |
| (1,2168) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HG2 | 14 | 0.42 | 0.23 | 0.44 |
| (1,3277) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA3 | 14 | 0.37 | 0.16 | 0.4 |
| (1,3277) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA3 | 14 | 0.37 | 0.16 | 0.4 |
| (1,3277) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA3 | 14 | 0.37 | 0.16 | 0.4 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG2 | 14 | 0.36 | 0.17 | 0.34 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG3 | 14 | 0.36 | 0.17 | 0.34 |
| (1,1258) | 1:163:A:GLN:HG2 | 1:164:A:GLY:HA3 | 14 | 0.35 | 0.14 | 0.35 |
| (1,1258) | 1:163:A:GLN:HG3 | 1:164:A:GLY:HA3 | 14 | 0.35 | 0.14 | 0.35 |
| (1,1331) | 1:70:A:ASP:HB3 | 1:72:A:THR:H | 14 | 0.31 | 0.13 | 0.32 |
| (1,606) | 1:137:A:GLN:H | 1:137:A:GLN:HG2 | 14 | 0.31 | 0.12 | 0.34 |
| (1,1604) | 1:61:A:VAL:HA | 1:62:A:GLU:HG2 | 14 | 0.29 | 0.11 | 0.24 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG21 | 14 | 0.29 | 0.13 | 0.24 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG22 | 14 | 0.29 | 0.13 | 0.24 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG23 | 14 | 0.29 | 0.13 | 0.24 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG21 | 14 | 0.29 | 0.13 | 0.24 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG22 | 14 | 0.29 | 0.13 | 0.24 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG23 | 14 | 0.29 | 0.13 | 0.24 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG21 | 14 | 0.29 | 0.13 | 0.24 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG22 | 14 | 0.29 | 0.13 | 0.24 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG23 | 14 | 0.29 | 0.13 | 0.24 |
| (1,2621) | 1:101:A:VAL:HG21 | 1:106:A:ASP:H | 14 | 0.29 | 0.18 | 0.26 |
| (1,2621) | 1:101:A:VAL:HG22 | 1:106:A:ASP:H | 14 | 0.29 | 0.18 | 0.26 |
| (1,2621) | 1:101:A:VAL:HG23 | 1:106:A:ASP:H | 14 | 0.29 | 0.18 | 0.26 |
| (1,216) | 1:34:A:TYR:H | 1:96:A:GLN:HE21 | 14 | 0.23 | 0.08 | 0.22 |
| (1,1474) | 1:161:A:ASN:HB2 | 1:161:A:ASN:HD22 | 14 | 0.22 | 0.09 | 0.18 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD1 | 14 | 0.14 | 0.01 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD2 | 14 | 0.14 | 0.01 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD1 | 14 | 0.14 | 0.01 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD2 | 14 | 0.14 | 0.01 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD1 | 14 | 0.14 | 0.01 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD2 | 14 | 0.14 | 0.01 | 0.14 |
| (1,3463) | 1:77:A:VAL:H | 1:125:A:TRP:HE3 | 14 | 0.13 | 0.01 | 0.13 |
| (1,175) | 1:87:A:ILE:HG21 | 1:113:A:ASP:H | 14 | 0.11 | 0.01 | 0.11 |
| (1,175) | 1:87:A:ILE:HG22 | 1:113:A:ASP:H | 14 | 0.11 | 0.01 | 0.11 |
| (1,175) | 1:87:A:ILE:HG23 | 1:113:A:ASP:H | 14 | 0.11 | 0.01 | 0.11 |
| (1,235) | 1:87:A:ILE:HG21 | 1:89:A:ALA:H | 14 | 0.11 | 0.0 | 0.11 |
| (1,235) | 1:87:A:ILE:HG22 | 1:89:A:ALA:H | 14 | 0.11 | 0.0 | 0.11 |
| (1,235) | 1:87:A:ILE:HG23 | 1:89:A:ALA:H | 14 | 0.11 | 0.0 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE1 | 13 | 1.2 | 0.68 | 1.26 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE2 | 13 | 1.2 | 0.68 | 1.26 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE3 | 13 | 1.2 | 0.68 | 1.26 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG21 | 13 | 1.18 | 0.52 | 1.1 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG22 | 13 | 1.18 | 0.52 | 1.1 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG23 | 13 | 1.18 | 0.52 | 1.1 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG21 | 13 | 1.18 | 0.52 | 1.1 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG22 | 13 | 1.18 | 0.52 | 1.1 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG23 | 13 | 1.18 | 0.52 | 1.1 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD1 | 13 | 0.7 | 0.35 | 0.7 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD2 | 13 | 0.7 | 0.35 | 0.7 |
| (1,128) | 1:12:A:LEU:HD11 | 1:159:A:GLN:H | 13 | 0.69 | 0.2 | 0.7 |
| (1,128) | 1:12:A:LEU:HD12 | 1:159:A:GLN:H | 13 | 0.69 | 0.2 | 0.7 |
| (1,128) | 1:12:A:LEU:HD13 | 1:159:A:GLN:H | 13 | 0.69 | 0.2 | 0.7 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB2 | 13 | 0.6 | 0.35 | 0.48 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB3 | 13 | 0.6 | 0.35 | 0.48 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG11 | 13 | 0.59 | 0.31 | 0.52 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG12 | 13 | 0.59 | 0.31 | 0.52 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG13 | 13 | 0.59 | 0.31 | 0.52 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG11 | 13 | 0.56 | 0.3 | 0.48 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG12 | 13 | 0.56 | 0.3 | 0.48 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG13 | 13 | 0.56 | 0.3 | 0.48 |
| (1,1813) | 1:160:A:LEU:HD21 | 1:180:A:THR:HB | 13 | 0.48 | 0.2 | 0.43 |
| (1,1813) | 1:160:A:LEU:HD22 | 1:180:A:THR:HB | 13 | 0.48 | 0.2 | 0.43 |
| (1,1813) | 1:160:A:LEU:HD23 | 1:180:A:THR:HB | 13 | 0.48 | 0.2 | 0.43 |
| (1,1867) | 1:37:A:GLU:HB2 | 1:38:A:GLU:HA | 13 | 0.46 | 0.13 | 0.52 |
| (1,1298) | 1:141:A:ALA:HA | 1:146:A:LEU:HB2 | 13 | 0.46 | 0.21 | 0.56 |
| (1,1931) | 1:62:A:GLU:HB2 | 1:63:A:PHE:HB3 | 13 | 0.45 | 0.14 | 0.49 |
| (1,1931) | 1:62:A:GLU:HB3 | 1:63:A:PHE:HB3 | 13 | 0.45 | 0.14 | 0.49 |
| (1,1686) | 1:99:A:GLN:HG3 | 1:100:A:THR:H | 13 | 0.44 | 0.1 | 0.43 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG11 | 13 | 0.41 | 0.24 | 0.27 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG12 | 13 | 0.41 | 0.24 | 0.27 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG13 | 13 | 0.41 | 0.24 | 0.27 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG11 | 13 | 0.41 | 0.2 | 0.37 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG12 | 13 | 0.41 | 0.2 | 0.37 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG13 | 13 | 0.41 | 0.2 | 0.37 |
| (1,2171) | 1:86:A:LYS:H | 1:87:A:ILE:HG12 | 13 | 0.4 | 0.17 | 0.42 |
| (1,438) | 1:60:A:HIS:HB2 | 1:75:A:TRP:H | 13 | 0.38 | 0.12 | 0.4 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD1 | 13 | 0.35 | 0.21 | 0.26 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD2 | 13 | 0.35 | 0.21 | 0.26 |
| (1,132) | 1:56:A:MET:HB2 | 1:57:A:THR:H | 13 | 0.33 | 0.13 | 0.37 |
| (1,2588) | 1:70:A:ASP:HA | 1:72:A:THR:H | 13 | 0.33 | 0.11 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,485) | 1:4:A:THR:H | 1:7:A:LYS:HB2 | 13 | 0.3 | 0.09 | 0.28 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG2 | 13 | 0.29 | 0.02 | 0.3 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG3 | 13 | 0.29 | 0.02 | 0.3 |
| (1,67) | 1:26:A:PHE:H | 1:59:A:TYR:H | 13 | 0.29 | 0.14 | 0.22 |
| (1,1698) | 1:136:A:GLN:HB2 | 1:136:A:GLN:HG2 | 13 | 0.28 | 0.06 | 0.29 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG21 | 13 | 0.28 | 0.07 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG22 | 13 | 0.28 | 0.07 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG23 | 13 | 0.28 | 0.07 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG21 | 13 | 0.28 | 0.07 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG22 | 13 | 0.28 | 0.07 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG23 | 13 | 0.28 | 0.07 | 0.33 |
| (1,2838) | 1:34:A:TYR:HE1 | 1:38:A:GLU:HA | 13 | 0.27 | 0.17 | 0.22 |
| (1,2838) | 1:34:A:TYR:HE2 | 1:38:A:GLU:HA | 13 | 0.27 | 0.17 | 0.22 |
| (1,1785) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD2 | 13 | 0.23 | 0.19 | 0.17 |
| (1,2118) | 1:10:A:ILE:HG13 | 1:159:A:GLN:H | 13 | 0.22 | 0.07 | 0.19 |
| (1,1930) | 1:186:A:GLU:HB3 | 1:187:A:LYS:H | 13 | 0.2 | 0.06 | 0.16 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG21 | 13 | 0.18 | 0.06 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG22 | 13 | 0.18 | 0.06 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG23 | 13 | 0.18 | 0.06 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG21 | 13 | 0.18 | 0.06 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG22 | 13 | 0.18 | 0.06 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG23 | 13 | 0.18 | 0.06 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG21 | 13 | 0.18 | 0.06 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG22 | 13 | 0.18 | 0.06 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG23 | 13 | 0.18 | 0.06 | 0.17 |
| (1,1832) | 1:124:A:ALA:HB1 | 1:130:A:VAL:HB | 13 | 0.16 | 0.05 | 0.15 |
| (1,1832) | 1:124:A:ALA:HB2 | 1:130:A:VAL:HB | 13 | 0.16 | 0.05 | 0.15 |
| (1,1832) | 1:124:A:ALA:HB3 | 1:130:A:VAL:HB | 13 | 0.16 | 0.05 | 0.15 |
| (1,1758) | 1:14:A:LYS:H | 1:14:A:LYS:HB3 | 13 | 0.15 | 0.03 | 0.15 |
| (1,300) | 1:130:A:VAL:HG21 | 1:131:A:LYS:H | 13 | 0.15 | 0.03 | 0.15 |
| (1,300) | 1:130:A:VAL:HG22 | 1:131:A:LYS:H | 13 | 0.15 | 0.03 | 0.15 |
| (1,300) | 1:130:A:VAL:HG23 | 1:131:A:LYS:H | 13 | 0.15 | 0.03 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE1 | 13 | 0.13 | 0.01 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE2 | 13 | 0.13 | 0.01 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE1 | 13 | 0.13 | 0.01 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE2 | 13 | 0.13 | 0.01 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE1 | 13 | 0.13 | 0.01 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE2 | 13 | 0.13 | 0.01 | 0.14 |
| (1,445) | 1:169:A:ASN:HD21 | 1:171:A:ASP:H | 13 | 0.11 | 0.0 | 0.11 |
| (1,1669) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HG2 | 12 | 0.68 | 0.33 | 0.74 |
| (1,1669) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HG2 | 12 | 0.68 | 0.33 | 0.74 |
| (1,1669) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HG2 | 12 | 0.68 | 0.33 | 0.74 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD11 | 12 | 0.53 | 0.29 | 0.5 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD12 | 12 | 0.53 | 0.29 | 0.5 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD13 | 12 | 0.53 | 0.29 | 0.5 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD11 | 12 | 0.53 | 0.29 | 0.5 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD12 | 12 | 0.53 | 0.29 | 0.5 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD13 | 12 | 0.53 | 0.29 | 0.5 |
| (1,2316) | 1:117:A:LYS:H | 1:117:A:LYS:HG2 | 12 | 0.51 | 0.14 | 0.52 |
| (1,2291) | 1:117:A:LYS:HG3 | 1:120:A:ASP:H | 12 | 0.49 | 0.19 | 0.46 |
| (1,1632) | 1:31:A:PRO:HA | 1:96:A:GLN:HG2 | 12 | 0.48 | 0.33 | 0.38 |
| (1,3112) | 1:67:A:LEU:HA | 1:70:A:ASP:HB3 | 12 | 0.42 | 0.12 | 0.39 |
| (1,2318) | 1:117:A:LYS:HG3 | 1:119:A:GLU:H | 12 | 0.41 | 0.01 | 0.41 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG21 | 12 | 0.36 | 0.15 | 0.34 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG22 | 12 | 0.36 | 0.15 | 0.34 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG23 | 12 | 0.36 | 0.15 | 0.34 |
| (1,1778) | 1:72:A:THR:HB | 1:73:A:GLN:HB3 | 12 | 0.34 | 0.17 | 0.32 |
| (1,78) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 12 | 0.32 | 0.1 | 0.29 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD21 | 12 | 0.32 | 0.15 | 0.36 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD22 | 12 | 0.32 | 0.15 | 0.36 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD23 | 12 | 0.32 | 0.15 | 0.36 |
| (1,2935) | 1:75:A:TRP:HA | 1:78:A:ALA:HA | 12 | 0.31 | 0.16 | 0.28 |
| (1,599) | 1:183:A:GLN:HB3 | 1:184:A:LEU:H | 12 | 0.23 | 0.08 | 0.24 |
| (1,555) | 1:174:A:VAL:HG21 | 1:178:A:ALA:H | 12 | 0.23 | 0.09 | 0.2 |
| (1,555) | 1:174:A:VAL:HG22 | 1:178:A:ALA:H | 12 | 0.23 | 0.09 | 0.2 |
| (1,555) | 1:174:A:VAL:HG23 | 1:178:A:ALA:H | 12 | 0.23 | 0.09 | 0.2 |
| (1,650) | 1:145:A:GLN:HA | 1:146:A:LEU:H | 12 | 0.2 | 0.04 | 0.21 |
| (1,3419) | 1:75:A:TRP:HB2 | 1:75:A:TRP:HD1 | 12 | 0.14 | 0.03 | 0.13 |
| (1,334) | 1:165:A:MET:HG2 | 1:166:A:ASP:H | 12 | 0.11 | 0.01 | 0.11 |
| (1,334) | 1:165:A:MET:HG3 | 1:166:A:ASP:H | 12 | 0.11 | 0.01 | 0.11 |
| (1,408) | 1:2:A:GLN:H | 1:3:A:ILE:H | 12 | 0.11 | 0.0 | 0.11 |
| (1,1715) | 1:133:A:LEU:H | 1:136:A:GLN:HG2 | 11 | 1.46 | 0.42 | 1.57 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE1 | 11 | 0.72 | 0.2 | 0.75 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE2 | 11 | 0.72 | 0.2 | 0.75 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB2 | 11 | 0.47 | 0.21 | 0.47 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB3 | 11 | 0.47 | 0.21 | 0.47 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB2 | 11 | 0.47 | 0.21 | 0.47 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB3 | 11 | 0.47 | 0.21 | 0.47 |
| (1,3297) | 1:23:A:LEU:HB2 | 1:153:A:TYR:H | 11 | 0.46 | 0.21 | 0.45 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB2 | 11 | 0.44 | 0.24 | 0.42 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB3 | 11 | 0.44 | 0.24 | 0.42 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB2 | 11 | 0.44 | 0.24 | 0.42 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB3 | 11 | 0.44 | 0.24 | 0.42 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB2 | 11 | 0.44 | 0.24 | 0.42 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB3 | 11 | 0.44 | 0.24 | 0.42 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG21 | 11 | 0.36 | 0.18 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG22 | 11 | 0.36 | 0.18 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG23 | 11 | 0.36 | 0.18 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG21 | 11 | 0.36 | 0.18 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG22 | 11 | 0.36 | 0.18 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG23 | 11 | 0.36 | 0.18 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG21 | 11 | 0.36 | 0.18 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG22 | 11 | 0.36 | 0.18 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG23 | 11 | 0.36 | 0.18 | 0.29 |
| (1,498) | 1:77:A:VAL:HG11 | 1:124:A:ALA:H | 11 | 0.31 | 0.09 | 0.33 |
| (1,498) | 1:77:A:VAL:HG12 | 1:124:A:ALA:H | 11 | 0.31 | 0.09 | 0.33 |
| (1,498) | 1:77:A:VAL:HG13 | 1:124:A:ALA:H | 11 | 0.31 | 0.09 | 0.33 |
| (1,1694) | 1:136:A:GLN:HG2 | 1:137:A:GLN:H | 11 | 0.3 | 0.08 | 0.34 |
| (1,2632) | 1:101:A:VAL:HG21 | 1:107:A:ILE:H | 11 | 0.29 | 0.2 | 0.26 |
| (1,2632) | 1:101:A:VAL:HG22 | 1:107:A:ILE:H | 11 | 0.29 | 0.2 | 0.26 |
| (1,2632) | 1:101:A:VAL:HG23 | 1:107:A:ILE:H | 11 | 0.29 | 0.2 | 0.26 |
| (1,2159) | 1:76:A:ALA:HA | 1:79:A:ILE:HG12 | 11 | 0.26 | 0.09 | 0.24 |
| (1,1526) | 1:63:A:PHE:HB2 | 1:64:A:LEU:H | 11 | 0.25 | 0.07 | 0.26 |
| (1,1040) | 1:52:A:GLU:HB3 | 1:53:A:GLY:H | 11 | 0.24 | 0.07 | 0.25 |
| (1,632) | 1:87:A:ILE:HG21 | 1:91:A:MET:H | 11 | 0.24 | 0.1 | 0.23 |
| (1,632) | 1:87:A:ILE:HG22 | 1:91:A:MET:H | 11 | 0.24 | 0.1 | 0.23 |
| (1,632) | 1:87:A:ILE:HG23 | 1:91:A:MET:H | 11 | 0.24 | 0.1 | 0.23 |
| (1,560) | 1:42:A:VAL:HG21 | 1:178:A:ALA:H | 11 | 0.23 | 0.09 | 0.21 |
| (1,560) | 1:42:A:VAL:HG22 | 1:178:A:ALA:H | 11 | 0.23 | 0.09 | 0.21 |
| (1,560) | 1:42:A:VAL:HG23 | 1:178:A:ALA:H | 11 | 0.23 | 0.09 | 0.21 |
| (1,1981) | 1:187:A:LYS:H | 1:187:A:LYS:HD3 | 11 | 0.21 | 0.06 | 0.21 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD21 | 11 | 0.2 | 0.07 | 0.2 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD22 | 11 | 0.2 | 0.07 | 0.2 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD23 | 11 | 0.2 | 0.07 | 0.2 |
| (1,1685) | 1:99:A:GLN:HA | 1:99:A:GLN:HG3 | 11 | 0.18 | 0.03 | 0.19 |
| (1,3461) | 1:75:A:TRP:HB3 | 1:75:A:TRP:HE3 | 11 | 0.14 | 0.03 | 0.14 |
| (1,62) | 1:102:A:GLN:H | 1:102:A:GLN:HG2 | 11 | 0.14 | 0.01 | 0.15 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE1 | 11 | 0.14 | 0.02 | 0.14 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE2 | 11 | 0.14 | 0.02 | 0.14 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE1 | 11 | 0.14 | 0.02 | 0.14 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE2 | 11 | 0.14 | 0.02 | 0.14 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE1 | 11 | 0.13 | 0.02 | 0.13 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE2 | 11 | 0.13 | 0.02 | 0.13 |
| (1,2484) | 1:183:A:GLN:HA | 1:183:A:GLN:HB2 | 11 | 0.12 | 0.01 | 0.11 |
| (1,3043) | 1:9:A:TYR:HD1 | 1:160:A:LEU:HA | 11 | 0.11 | 0.0 | 0.11 |
| (1,3043) | 1:9:A:TYR:HD2 | 1:160:A:LEU:HA | 11 | 0.11 | 0.0 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2017) | 1:117:A:LYS:HD3 | 1:120:A:ASP:H | 10 | 1.11 | 0.34 | 1.26 |
| (1,2945) | 1:23:A:LEU:HD21 | 1:58:A:LYS:HA | 10 | 0.81 | 0.33 | 0.89 |
| (1,2945) | 1:23:A:LEU:HD22 | 1:58:A:LYS:HA | 10 | 0.81 | 0.33 | 0.89 |
| (1,2945) | 1:23:A:LEU:HD23 | 1:58:A:LYS:HA | 10 | 0.81 | 0.33 | 0.89 |
| (1,1697) | 1:132:A:SER:HB2 | 1:136:A:GLN:HG2 | 10 | 0.8 | 0.33 | 0.8 |
| (1,1697) | 1:132:A:SER:HB3 | 1:136:A:GLN:HG2 | 10 | 0.8 | 0.33 | 0.8 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG21 | 10 | 0.46 | 0.25 | 0.46 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG22 | 10 | 0.46 | 0.25 | 0.46 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG23 | 10 | 0.46 | 0.25 | 0.46 |
| (1,1213) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE21 | 10 | 0.45 | 0.33 | 0.38 |
| (1,1213) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE21 | 10 | 0.45 | 0.33 | 0.38 |
| (1,1213) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE21 | 10 | 0.45 | 0.33 | 0.38 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE1 | 10 | 0.44 | 0.18 | 0.41 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE2 | 10 | 0.44 | 0.18 | 0.41 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE1 | 10 | 0.44 | 0.18 | 0.41 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE2 | 10 | 0.44 | 0.18 | 0.41 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE1 | 10 | 0.44 | 0.18 | 0.41 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE2 | 10 | 0.44 | 0.18 | 0.41 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB2 | 10 | 0.43 | 0.12 | 0.48 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB3 | 10 | 0.43 | 0.12 | 0.48 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE1 | 10 | 0.35 | 0.19 | 0.3 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE2 | 10 | 0.35 | 0.19 | 0.3 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE1 | 10 | 0.35 | 0.19 | 0.3 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE2 | 10 | 0.35 | 0.19 | 0.3 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE1 | 10 | 0.35 | 0.19 | 0.3 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE2 | 10 | 0.35 | 0.19 | 0.3 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG21 | 10 | 0.34 | 0.16 | 0.36 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG22 | 10 | 0.34 | 0.16 | 0.36 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG23 | 10 | 0.34 | 0.16 | 0.36 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG21 | 10 | 0.34 | 0.16 | 0.36 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG22 | 10 | 0.34 | 0.16 | 0.36 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG23 | 10 | 0.34 | 0.16 | 0.36 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG21 | 10 | 0.34 | 0.16 | 0.36 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG22 | 10 | 0.34 | 0.16 | 0.36 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG23 | 10 | 0.34 | 0.16 | 0.36 |
| (1,259) | 1:69:A:LYS:HD2 | 1:70:A:ASP:H | 10 | 0.33 | 0.12 | 0.35 |
| (1,2072) | 1:93:A:GLU:HA | 1:97:A:LYS:HD2 | 10 | 0.2 | 0.06 | 0.19 |
| (1,2622) | 1:149:A:VAL:HA | 1:151:A:ALA:H | 10 | 0.19 | 0.06 | 0.18 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD21 | 10 | 0.16 | 0.04 | 0.14 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD22 | 10 | 0.16 | 0.04 | 0.14 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD23 | 10 | 0.16 | 0.04 | 0.14 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE1 | 10 | 0.13 | 0.01 | 0.13 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE2 | 10 | 0.13 | 0.01 | 0.13 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE1 | 10 | 0.12 | 0.01 | 0.12 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE2 | 10 | 0.12 | 0.01 | 0.12 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE3 | 10 | 0.12 | 0.01 | 0.12 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE1 | 10 | 0.12 | 0.01 | 0.12 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE2 | 10 | 0.12 | 0.01 | 0.12 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE3 | 10 | 0.12 | 0.01 | 0.12 |
| (1,456) | 1:60:A:HIS:HB3 | 1:75:A:TRP:H | 10 | 0.11 | 0.01 | 0.11 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB1 | 10 | 0.11 | 0.01 | 0.11 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB2 | 10 | 0.11 | 0.01 | 0.11 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB3 | 10 | 0.11 | 0.01 | 0.11 |
| (1,2304) | 1:132:A:SER:HA | 1:136:A:GLN:HG2 | 9 | 0.92 | 0.37 | 1.04 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD21 | 9 | 0.66 | 0.28 | 0.75 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD22 | 9 | 0.66 | 0.28 | 0.75 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD23 | 9 | 0.66 | 0.28 | 0.75 |
| (1,2392) | 1:31:A:PRO:HA | 1:34:A:TYR:HA | 9 | 0.49 | 0.38 | 0.31 |
| (1,1606) | 1:52:A:GLU:HG2 | 1:53:A:GLY:HA3 | 9 | 0.38 | 0.12 | 0.38 |
| (1,1606) | 1:52:A:GLU:HG3 | 1:53:A:GLY:HA3 | 9 | 0.38 | 0.12 | 0.38 |
| (1,2756) | 1:146:A:LEU:HA | 1:147:A:GLN:H | 9 | 0.35 | 0.01 | 0.36 |
| (1,241) | 1:70:A:ASP:HB2 | 1:74:A:ALA:H | 9 | 0.28 | 0.1 | 0.27 |
| (1,1294) | 1:71:A:LEU:HB2 | 1:74:A:ALA:H | 9 | 0.25 | 0.11 | 0.19 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG2 | 9 | 0.25 | 0.1 | 0.22 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG3 | 9 | 0.25 | 0.1 | 0.22 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD1 | 9 | 0.23 | 0.09 | 0.21 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD2 | 9 | 0.23 | 0.09 | 0.21 |
| (1,1513) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB2 | 9 | 0.23 | 0.07 | 0.21 |
| (1,1513) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB2 | 9 | 0.23 | 0.07 | 0.21 |
| (1,1513) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB2 | 9 | 0.23 | 0.07 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG21 | 9 | 0.22 | 0.1 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG22 | 9 | 0.22 | 0.1 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG23 | 9 | 0.22 | 0.1 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG21 | 9 | 0.22 | 0.1 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG22 | 9 | 0.22 | 0.1 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG23 | 9 | 0.22 | 0.1 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG21 | 9 | 0.22 | 0.1 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG22 | 9 | 0.22 | 0.1 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG23 | 9 | 0.22 | 0.1 | 0.21 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE1 | 9 | 0.21 | 0.06 | 0.22 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE2 | 9 | 0.21 | 0.06 | 0.22 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE3 | 9 | 0.21 | 0.06 | 0.22 |
| (1,40) | 1:5:A:ASP:H | 1:7:A:LYS:HB2 | 9 | 0.21 | 0.06 | 0.19 |
| (1,815) | 1:91:A:MET:HB2 | 1:93:A:GLU:H | 9 | 0.19 | 0.07 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD11 | 9 | 0.14 | 0.02 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD12 | 9 | 0.14 | 0.02 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD13 | 9 | 0.14 | 0.02 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD11 | 9 | 0.14 | 0.02 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD12 | 9 | 0.14 | 0.02 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD13 | 9 | 0.14 | 0.02 | 0.14 |
| (1,3336) | 1:92:A:PHE:HD1 | 1:96:A:GLN:HG2 | 9 | 0.13 | 0.01 | 0.13 |
| (1,3336) | 1:92:A:PHE:HD2 | 1:96:A:GLN:HG2 | 9 | 0.13 | 0.01 | 0.13 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD1 | 9 | 0.12 | 0.01 | 0.12 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD2 | 9 | 0.12 | 0.01 | 0.12 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG11 | 8 | 0.82 | 0.25 | 0.89 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG12 | 8 | 0.82 | 0.25 | 0.89 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG13 | 8 | 0.82 | 0.25 | 0.89 |
| (1,1427) | 1:143:A:ASP:HB2 | 1:145:A:GLN:HE22 | 8 | 0.78 | 0.51 | 0.68 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE1 | 8 | 0.52 | 0.33 | 0.7 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE2 | 8 | 0.52 | 0.33 | 0.7 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB2 | 8 | 0.52 | 0.12 | 0.51 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB3 | 8 | 0.52 | 0.12 | 0.51 |
| (1,3252) | 1:29:A:TYR:HD1 | 1:68:A:GLY:HA3 | 8 | 0.38 | 0.29 | 0.34 |
| (1,3252) | 1:29:A:TYR:HD2 | 1:68:A:GLY:HA3 | 8 | 0.38 | 0.29 | 0.34 |
| (1,1366) | 1:34:A:TYR:HE1 | 1:97:A:LYS:HE3 | 8 | 0.37 | 0.22 | 0.26 |
| (1,1366) | 1:34:A:TYR:HE2 | 1:97:A:LYS:HE3 | 8 | 0.37 | 0.22 | 0.26 |
| (1,3274) | 1:118:A:GLY:HA3 | 1:121:A:TYR:H | 8 | 0.34 | 0.2 | 0.28 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB2 | 8 | 0.33 | 0.18 | 0.3 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB3 | 8 | 0.33 | 0.18 | 0.3 |
| (1,587) | 1:46:A:VAL:HG21 | 1:47:A:ARG:H | 8 | 0.29 | 0.11 | 0.24 |
| (1,587) | 1:46:A:VAL:HG22 | 1:47:A:ARG:H | 8 | 0.29 | 0.11 | 0.24 |
| (1,587) | 1:46:A:VAL:HG23 | 1:47:A:ARG:H | 8 | 0.29 | 0.11 | 0.24 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG11 | 8 | 0.29 | 0.13 | 0.29 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG12 | 8 | 0.29 | 0.13 | 0.29 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG13 | 8 | 0.29 | 0.13 | 0.29 |
| (1,2581) | 1:52:A:GLU:HA | 1:53:A:GLY:HA3 | 8 | 0.27 | 0.09 | 0.28 |
| (1,1265) | 1:64:A:LEU:HB3 | 1:65:A:GLY:HA2 | 8 | 0.23 | 0.11 | 0.18 |
| (1,165) | 1:67:A:LEU:H | 1:69:A:LYS:H | 8 | 0.2 | 0.08 | 0.18 |
| (1,938) | 1:112:A:VAL:HG11 | 1:118:A:GLY:H | 8 | 0.18 | 0.06 | 0.16 |
| (1,938) | 1:112:A:VAL:HG12 | 1:118:A:GLY:H | 8 | 0.18 | 0.06 | 0.16 |
| (1,938) | 1:112:A:VAL:HG13 | 1:118:A:GLY:H | 8 | 0.18 | 0.06 | 0.16 |
| (1,1730) | 1:55:A:LYS:H | 1:55:A:LYS:HB3 | 8 | 0.18 | 0.04 | 0.18 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB2 | 8 | 0.17 | 0.03 | 0.18 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB3 | 8 | 0.17 | 0.03 | 0.18 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB1 | 8 | 0.11 | 0.01 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB2 | 8 | 0.11 | 0.01 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB3 | 8 | 0.11 | 0.01 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB1 | 8 | 0.11 | 0.01 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB2 | 8 | 0.11 | 0.01 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB3 | 8 | 0.11 | 0.01 | 0.12 |
| (1,2441) | 1:119:A:GLU:HA | 1:122:A:ASP:HB3 | 7 | 1.45 | 0.21 | 1.47 |
| (1,416) | 1:122:A:ASP:HB3 | 1:123:A:ALA:H | 7 | 0.73 | 0.12 | 0.7 |
| (1,1358) | 1:179:A:ASP:HB3 | 1:183:A:GLN:HE21 | 7 | 0.66 | 0.18 | 0.64 |
| (1,2016) | 1:117:A:LYS:HD3 | 1:119:A:GLU:H | 7 | 0.59 | 0.21 | 0.55 |
| (1,3415) | 1:59:A:TYR:HD1 | 1:137:A:GLN:HG3 | 7 | 0.55 | 0.31 | 0.52 |
| (1,3415) | 1:59:A:TYR:HD2 | 1:137:A:GLN:HG3 | 7 | 0.55 | 0.31 | 0.52 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG21 | 7 | 0.44 | 0.05 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG22 | 7 | 0.44 | 0.05 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG23 | 7 | 0.44 | 0.05 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG21 | 7 | 0.44 | 0.05 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG22 | 7 | 0.44 | 0.05 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG23 | 7 | 0.44 | 0.05 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG21 | 7 | 0.44 | 0.05 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG22 | 7 | 0.44 | 0.05 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG23 | 7 | 0.44 | 0.05 | 0.46 |
| (1,578) | 1:122:A:ASP:H | 1:122:A:ASP:HB3 | 7 | 0.41 | 0.02 | 0.41 |
| (1,337) | 1:166:A:ASP:H | 1:176:A:GLN:HE21 | 7 | 0.4 | 0.2 | 0.38 |
| (1,1426) | 1:143:A:ASP:HB2 | 1:144:A:LEU:HG | 7 | 0.37 | 0.29 | 0.22 |
| (1,3481) | 1:29:A:TYR:HE1 | 1:67:A:LEU:HA | 7 | 0.33 | 0.17 | 0.36 |
| (1,3481) | 1:29:A:TYR:HE2 | 1:67:A:LEU:HA | 7 | 0.33 | 0.17 | 0.36 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG21 | 7 | 0.32 | 0.22 | 0.23 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG22 | 7 | 0.32 | 0.22 | 0.23 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG23 | 7 | 0.32 | 0.22 | 0.23 |
| (1,83) | 1:6:A:GLY:H | 1:11:A:THR:H | 7 | 0.32 | 0.14 | 0.25 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB1 | 7 | 0.31 | 0.1 | 0.36 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB2 | 7 | 0.31 | 0.1 | 0.36 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB3 | 7 | 0.31 | 0.1 | 0.36 |
| (1,401) | 1:117:A:LYS:HB2 | 1:120:A:ASP:H | 7 | 0.31 | 0.09 | 0.29 |
| (1,2943) | 1:3:A:ILE:HG21 | 1:8:A:GLN:HG3 | 7 | 0.26 | 0.12 | 0.23 |
| (1,2943) | 1:3:A:ILE:HG22 | 1:8:A:GLN:HG3 | 7 | 0.26 | 0.12 | 0.23 |
| (1,2943) | 1:3:A:ILE:HG23 | 1:8:A:GLN:HG3 | 7 | 0.26 | 0.12 | 0.23 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD11 | 7 | 0.24 | 0.12 | 0.21 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD12 | 7 | 0.24 | 0.12 | 0.21 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD13 | 7 | 0.24 | 0.12 | 0.21 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD11 | 7 | 0.24 | 0.12 | 0.21 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD12 | 7 | 0.24 | 0.12 | 0.21 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD13 | 7 | 0.24 | 0.12 | 0.21 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD11 | 7 | 0.24 | 0.12 | 0.21 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD12 | 7 | 0.24 | 0.12 | 0.21 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD13 | 7 | 0.24 | 0.12 | 0.21 |
| (1,1699) | 1:135:A:ALA:HB1 | 1:136:A:GLN:HG2 | 7 | 0.24 | 0.08 | 0.24 |
| (1,1699) | 1:135:A:ALA:HB2 | 1:136:A:GLN:HG2 | 7 | 0.24 | 0.08 | 0.24 |
| (1,1699) | 1:135:A:ALA:HB3 | 1:136:A:GLN:HG2 | 7 | 0.24 | 0.08 | 0.24 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG11 | 7 | 0.22 | 0.12 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG12 | 7 | 0.22 | 0.12 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG13 | 7 | 0.22 | 0.12 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG11 | 7 | 0.22 | 0.12 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG12 | 7 | 0.22 | 0.12 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG13 | 7 | 0.22 | 0.12 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG11 | 7 | 0.22 | 0.12 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG12 | 7 | 0.22 | 0.12 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG13 | 7 | 0.22 | 0.12 | 0.19 |
| (1,577) | 1:121:A:TYR:HB2 | 1:122:A:ASP:H | 7 | 0.21 | 0.06 | 0.22 |
| (1,3305) | 1:38:A:GLU:H | 1:41:A:HIS:HE1 | 7 | 0.14 | 0.01 | 0.15 |
| (1,1693) | 1:136:A:GLN:H | 1:136:A:GLN:HG2 | 7 | 0.13 | 0.01 | 0.14 |
| (1,3422) | 1:60:A:HIS:H | 1:75:A:TRP:HD1 | 7 | 0.13 | 0.01 | 0.13 |
| (1,809) | 1:179:A:ASP:HA | 1:180:A:THR:H | 7 | 0.12 | 0.02 | 0.11 |
| (1,3388) | 1:34:A:TYR:HD1 | 1:92:A:PHE:HA | 7 | 0.12 | 0.01 | 0.11 |
| (1,3388) | 1:34:A:TYR:HD2 | 1:92:A:PHE:HA | 7 | 0.12 | 0.01 | 0.11 |
| (1,1587) | 1:51:A:PRO:HA | 1:52:A:GLU:HG2 | 7 | 0.11 | 0.0 | 0.11 |
| (1,1587) | 1:51:A:PRO:HA | 1:52:A:GLU:HG3 | 7 | 0.11 | 0.0 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG21 | 7 | 0.11 | 0.0 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG22 | 7 | 0.11 | 0.0 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG23 | 7 | 0.11 | 0.0 | 0.11 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE1 | 6 | 0.82 | 0.07 | 0.81 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE2 | 6 | 0.82 | 0.07 | 0.81 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE3 | 6 | 0.82 | 0.07 | 0.81 |
| (1,1577) | 1:152:A:MET:HB3 | 1:160:A:LEU:HB2 | 6 | 0.81 | 0.08 | 0.81 |
| (1,1545) | 1:186:A:GLU:HG3 | 1:187:A:LYS:HD3 | 6 | 0.78 | 0.66 | 0.47 |
| (1,242) | 1:145:A:GLN:HE21 | 1:147:A:GLN:H | 6 | 0.76 | 0.23 | 0.67 |
| (1,1084) | 1:37:A:GLU:HG3 | 1:38:A:GLU:H | 6 | 0.68 | 0.15 | 0.62 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD11 | 6 | 0.61 | 0.26 | 0.72 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD12 | 6 | 0.61 | 0.26 | 0.72 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD13 | 6 | 0.61 | 0.26 | 0.72 |
| (1,285) | 1:152:A:MET:H | 1:152:A:MET:HB3 | 6 | 0.38 | 0.07 | 0.36 |
| (1,1916) | 1:91:A:MET:HB2 | 1:92:A:PHE:HE1 | 6 | 0.36 | 0.56 | 0.11 |
| (1,1916) | 1:91:A:MET:HB2 | 1:92:A:PHE:HE2 | 6 | 0.36 | 0.56 | 0.11 |
| (1,1603) | 1:62:A:GLU:HG2 | 1:63:A:PHE:H | 6 | 0.34 | 0.12 | 0.32 |
| (1,799) | 1:49:A:LYS:HG2 | 1:179:A:ASP:H | 6 | 0.33 | 0.15 | 0.29 |
| (1,799) | 1:49:A:LYS:HG3 | 1:179:A:ASP:H | 6 | 0.33 | 0.15 | 0.29 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1563) | 1:152:A:MET:HB3 | 1:160:A:LEU:HB3 | 6 | 0.32 | 0.03 | 0.34 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD21 | 6 | 0.28 | 0.1 | 0.25 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD22 | 6 | 0.28 | 0.1 | 0.25 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD23 | 6 | 0.28 | 0.1 | 0.25 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG11 | 6 | 0.19 | 0.05 | 0.18 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG12 | 6 | 0.19 | 0.05 | 0.18 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG13 | 6 | 0.19 | 0.05 | 0.18 |
| (1,1915) | 1:186:A:GLU:HB2 | 1:187:A:LYS:H | 6 | 0.17 | 0.03 | 0.17 |
| (1,3407) | 1:59:A:TYR:HD1 | 1:60:A:HIS:H | 6 | 0.14 | 0.01 | 0.14 |
| (1,3407) | 1:59:A:TYR:HD2 | 1:60:A:HIS:H | 6 | 0.14 | 0.01 | 0.14 |
| (1,936) | 1:117:A:LYS:HG3 | 1:118:A:GLY:H | 6 | 0.13 | 0.05 | 0.12 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD11 | 6 | 0.12 | 0.01 | 0.12 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD12 | 6 | 0.12 | 0.01 | 0.12 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD13 | 6 | 0.12 | 0.01 | 0.12 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD11 | 6 | 0.11 | 0.01 | 0.11 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD12 | 6 | 0.11 | 0.01 | 0.11 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD13 | 6 | 0.11 | 0.01 | 0.11 |
| (1,2880) | 1:135:A:ALA:HA | 1:138:A:GLU:HB2 | 5 | 1.8 | 0.09 | 1.84 |
| (1,3107) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HB2 | 5 | 1.69 | 0.1 | 1.73 |
| (1,3107) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HB2 | 5 | 1.69 | 0.1 | 1.73 |
| (1,3107) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HB2 | 5 | 1.69 | 0.1 | 1.73 |
| (1,1262) | 1:29:A:TYR:HB3 | 1:64:A:LEU:HB2 | 5 | 0.72 | 0.29 | 0.78 |
| (1,1432) | 1:85:A:ASP:HB3 | 1:86:A:LYS:HG2 | 5 | 0.71 | 0.44 | 0.53 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE1 | 5 | 0.66 | 0.04 | 0.68 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE2 | 5 | 0.66 | 0.04 | 0.68 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE3 | 5 | 0.66 | 0.04 | 0.68 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG21 | 5 | 0.44 | 0.24 | 0.55 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG22 | 5 | 0.44 | 0.24 | 0.55 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG23 | 5 | 0.44 | 0.24 | 0.55 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG21 | 5 | 0.44 | 0.24 | 0.55 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG22 | 5 | 0.44 | 0.24 | 0.55 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG23 | 5 | 0.44 | 0.24 | 0.55 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG21 | 5 | 0.44 | 0.24 | 0.55 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG22 | 5 | 0.44 | 0.24 | 0.55 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG23 | 5 | 0.44 | 0.24 | 0.55 |
| (1,3495) | 1:23:A:LEU:HD21 | 1:59:A:TYR:HE1 | 5 | 0.44 | 0.29 | 0.32 |
| (1,3495) | 1:23:A:LEU:HD21 | 1:59:A:TYR:HE2 | 5 | 0.44 | 0.29 | 0.32 |
| (1,3495) | 1:23:A:LEU:HD22 | 1:59:A:TYR:HE1 | 5 | 0.44 | 0.29 | 0.32 |
| (1,3495) | 1:23:A:LEU:HD22 | 1:59:A:TYR:HE2 | 5 | 0.44 | 0.29 | 0.32 |
| (1,3495) | 1:23:A:LEU:HD23 | 1:59:A:TYR:HE1 | 5 | 0.44 | 0.29 | 0.32 |
| (1,3495) | 1:23:A:LEU:HD23 | 1:59:A:TYR:HE2 | 5 | 0.44 | 0.29 | 0.32 |
| (1,1185) | 1:29:A:TYR:HE1 | 1:68:A:GLY:H | 5 | 0.41 | 0.13 | 0.34 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1185) | 1:29:A:TYR:HE2 | 1:68:A:GLY:H | 5 | 0.41 | 0.13 | 0.34 |
| (1,1485) | 1:28:A:PHE:HB2 | 1:95:A:VAL:HB | 5 | 0.4 | 0.09 | 0.38 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD21 | 5 | 0.34 | 0.15 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD22 | 5 | 0.34 | 0.15 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD23 | 5 | 0.34 | 0.15 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD21 | 5 | 0.34 | 0.15 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD22 | 5 | 0.34 | 0.15 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD23 | 5 | 0.34 | 0.15 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD21 | 5 | 0.34 | 0.15 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD22 | 5 | 0.34 | 0.15 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD23 | 5 | 0.34 | 0.15 | 0.36 |
| (1,1624) | 1:33:A:CYS:HA | 1:150:A:PRO:HB2 | 5 | 0.29 | 0.16 | 0.21 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB1 | 5 | 0.27 | 0.14 | 0.31 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB2 | 5 | 0.27 | 0.14 | 0.31 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB3 | 5 | 0.27 | 0.14 | 0.31 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB1 | 5 | 0.27 | 0.14 | 0.31 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB2 | 5 | 0.27 | 0.14 | 0.31 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB3 | 5 | 0.27 | 0.14 | 0.31 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB1 | 5 | 0.27 | 0.14 | 0.31 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB2 | 5 | 0.27 | 0.14 | 0.31 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB3 | 5 | 0.27 | 0.14 | 0.31 |
| (1,1354) | 1:73:A:GLN:HE22 | 1:131:A:LYS:HE2 | 5 | 0.25 | 0.25 | 0.11 |
| (1,1354) | 1:73:A:GLN:HE22 | 1:131:A:LYS:HE3 | 5 | 0.25 | 0.25 | 0.11 |
| (1,1744) | 1:134:A:VAL:HA | 1:137:A:GLN:HG2 | 5 | 0.25 | 0.04 | 0.25 |
| (1,2474) | 1:83:A:VAL:HA | 1:84:A:GLU:HB2 | 5 | 0.22 | 0.14 | 0.16 |
| (1,1873) | 1:46:A:VAL:HA | 1:49:A:LYS:HB3 | 5 | 0.22 | 0.1 | 0.2 |
| (1,2908) | 1:175:A:ALA:HA | 1:178:A:ALA:H | 5 | 0.21 | 0.08 | 0.19 |
| (1,1792) | 1:56:A:MET:HB2 | 1:56:A:MET:HG3 | 5 | 0.21 | 0.03 | 0.21 |
| (1,1450) | 1:42:A:VAL:HA | 1:45:A:ASN:HB3 | 5 | 0.19 | 0.08 | 0.15 |
| (1,3523) | 1:73:A:GLN:HE21 | 1:125:A:TRP:HZ2 | 5 | 0.19 | 0.06 | 0.17 |
| (1,3398) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HG2 | 5 | 0.14 | 0.02 | 0.14 |
| (1,3398) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HG3 | 5 | 0.14 | 0.02 | 0.14 |
| (1,3398) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HG2 | 5 | 0.14 | 0.02 | 0.14 |
| (1,3398) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HG3 | 5 | 0.14 | 0.02 | 0.14 |
| (1,3404) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HB2 | 5 | 0.13 | 0.02 | 0.14 |
| (1,3404) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HB3 | 5 | 0.13 | 0.02 | 0.14 |
| (1,3404) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HB2 | 5 | 0.13 | 0.02 | 0.14 |
| (1,3404) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HB3 | 5 | 0.13 | 0.02 | 0.14 |
| (1,3325) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HD1 | 5 | 0.13 | 0.01 | 0.12 |
| (1,3325) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HD2 | 5 | 0.13 | 0.01 | 0.12 |
| (1,3325) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HD1 | 5 | 0.13 | 0.01 | 0.12 |
| (1,3325) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HD2 | 5 | 0.13 | 0.01 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3325) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HD1 | 5 | 0.13 | 0.01 | 0.12 |
| (1,3325) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HD2 | 5 | 0.13 | 0.01 | 0.12 |
| (1,3428) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HA | 5 | 0.12 | 0.0 | 0.12 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE1 | 5 | 0.11 | 0.01 | 0.11 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE2 | 5 | 0.11 | 0.01 | 0.11 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE3 | 5 | 0.11 | 0.01 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB1 | 5 | 0.11 | 0.01 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB2 | 5 | 0.11 | 0.01 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB3 | 5 | 0.11 | 0.01 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB1 | 5 | 0.11 | 0.01 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB2 | 5 | 0.11 | 0.01 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB3 | 5 | 0.11 | 0.01 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD11 | 5 | 0.11 | 0.01 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD12 | 5 | 0.11 | 0.01 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD13 | 5 | 0.11 | 0.01 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD21 | 5 | 0.11 | 0.01 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD22 | 5 | 0.11 | 0.01 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD23 | 5 | 0.11 | 0.01 | 0.11 |
| (1,1859) | 1:103:A:SER:HB2 | 1:104:A:VAL:HB | 4 | 1.14 | 0.1 | 1.19 |
| (1,763) | 1:103:A:SER:HB2 | 1:106:A:ASP:H | 4 | 0.83 | 0.35 | 0.88 |
| (1,1641) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HB | 4 | 0.78 | 0.74 | 0.56 |
| (1,1641) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HB | 4 | 0.78 | 0.74 | 0.56 |
| (1,1641) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HB | 4 | 0.78 | 0.74 | 0.56 |
| (1,1963) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HD2 | 4 | 0.71 | 0.39 | 0.76 |
| (1,1963) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HD3 | 4 | 0.71 | 0.39 | 0.76 |
| (1,1141) | 1:126:A:ASN:H | 1:127:A:SER:HB3 | 4 | 0.65 | 0.45 | 0.66 |
| (1,1137) | 1:126:A:ASN:H | 1:126:A:ASN:HB3 | 4 | 0.62 | 0.02 | 0.62 |
| (1,2456) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HA | 4 | 0.55 | 0.1 | 0.57 |
| (1,2456) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HA | 4 | 0.55 | 0.1 | 0.57 |
| (1,2456) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HA | 4 | 0.55 | 0.1 | 0.57 |
| (1,530) | 1:128:A:PHE:HB3 | 1:129:A:VAL:H | 4 | 0.55 | 0.01 | 0.55 |
| (1,111) | 1:103:A:SER:HB2 | 1:105:A:ALA:H | 4 | 0.48 | 0.17 | 0.46 |
| (1,1547) | 1:152:A:MET:HB3 | 1:160:A:LEU:HD11 | 4 | 0.44 | 0.16 | 0.51 |
| (1,1547) | 1:152:A:MET:HB3 | 1:160:A:LEU:HD12 | 4 | 0.44 | 0.16 | 0.51 |
| (1,1547) | 1:152:A:MET:HB3 | 1:160:A:LEU:HD13 | 4 | 0.44 | 0.16 | 0.51 |
| (1,3276) | 1:118:A:GLY:HA3 | 1:121:A:TYR:HB3 | 4 | 0.42 | 0.12 | 0.49 |
| (1,3076) | 1:47:A:ARG:HG3 | 1:56:A:MET:HE1 | 4 | 0.42 | 0.32 | 0.36 |
| (1,3076) | 1:47:A:ARG:HG3 | 1:56:A:MET:HE2 | 4 | 0.42 | 0.32 | 0.36 |
| (1,3076) | 1:47:A:ARG:HG3 | 1:56:A:MET:HE3 | 4 | 0.42 | 0.32 | 0.36 |
| (1,492) | 1:138:A:GLU:HB2 | 1:140:A:ALA:H | 4 | 0.34 | 0.17 | 0.28 |
| (1,3250) | 1:68:A:GLY:HA3 | 1:71:A:LEU:HB2 | 4 | 0.34 | 0.07 | 0.35 |
| (1,553) | 1:42:A:VAL:HG21 | 1:46:A:VAL:H | 4 | 0.33 | 0.25 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,553) | 1:42:A:VAL:HG22 | 1:46:A:VAL:H | 4 | 0.33 | 0.25 | 0.22 |
| (1,553) | 1:42:A:VAL:HG23 | 1:46:A:VAL:H | 4 | 0.33 | 0.25 | 0.22 |
| (1,1843) | 1:60:A:HIS:HB2 | 1:72:A:THR:HA | 4 | 0.32 | 0.12 | 0.35 |
| (1,3420) | 1:60:A:HIS:HB3 | 1:75:A:TRP:HD1 | 4 | 0.32 | 0.11 | 0.29 |
| (1,1935) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HA | 4 | 0.3 | 0.07 | 0.3 |
| (1,185) | 1:59:A:TYR:HB2 | 1:60:A:HIS:H | 4 | 0.26 | 0.12 | 0.28 |
| (1,1116) | 1:61:A:VAL:HG11 | 1:63:A:PHE:H | 4 | 0.26 | 0.12 | 0.24 |
| (1,1116) | 1:61:A:VAL:HG12 | 1:63:A:PHE:H | 4 | 0.26 | 0.12 | 0.24 |
| (1,1116) | 1:61:A:VAL:HG13 | 1:63:A:PHE:H | 4 | 0.26 | 0.12 | 0.24 |
| (1,3230) | 1:87:A:ILE:HA | 1:90:A:PRO:HD3 | 4 | 0.24 | 0.14 | 0.2 |
| (1,1215) | 1:73:A:GLN:HE21 | 1:77:A:VAL:HG21 | 4 | 0.24 | 0.12 | 0.2 |
| (1,1215) | 1:73:A:GLN:HE21 | 1:77:A:VAL:HG22 | 4 | 0.24 | 0.12 | 0.2 |
| (1,1215) | 1:73:A:GLN:HE21 | 1:77:A:VAL:HG23 | 4 | 0.24 | 0.12 | 0.2 |
| (1,3229) | 1:88:A:THR:H | 1:90:A:PRO:HD3 | 4 | 0.23 | 0.05 | 0.22 |
| (1,1825) | 1:117:A:LYS:HB3 | 1:120:A:ASP:H | 4 | 0.22 | 0.18 | 0.12 |
| (1,3) | 1:152:A:MET:HB3 | 1:160:A:LEU:H | 4 | 0.22 | 0.05 | 0.21 |
| (1,380) | 1:138:A:GLU:H | 1:138:A:GLU:HG3 | 4 | 0.2 | 0.05 | 0.2 |
| (1,3389) | 1:128:A:PHE:HD2 | 1:131:A:LYS:HB2 | 4 | 0.16 | 0.0 | 0.16 |
| (1,3389) | 1:128:A:PHE:HD2 | 1:131:A:LYS:HB3 | 4 | 0.16 | 0.0 | 0.16 |
| (1,3053) | 1:172:A:VAL:HG21 | 1:175:A:ALA:HB1 | 4 | 0.15 | 0.02 | 0.15 |
| (1,3053) | 1:172:A:VAL:HG21 | 1:175:A:ALA:HB2 | 4 | 0.15 | 0.02 | 0.15 |
| (1,3053) | 1:172:A:VAL:HG21 | 1:175:A:ALA:HB3 | 4 | 0.15 | 0.02 | 0.15 |
| (1,3053) | 1:172:A:VAL:HG22 | 1:175:A:ALA:HB1 | 4 | 0.15 | 0.02 | 0.15 |
| (1,3053) | 1:172:A:VAL:HG22 | 1:175:A:ALA:HB2 | 4 | 0.15 | 0.02 | 0.15 |
| (1,3053) | 1:172:A:VAL:HG22 | 1:175:A:ALA:HB3 | 4 | 0.15 | 0.02 | 0.15 |
| (1,3053) | 1:172:A:VAL:HG23 | 1:175:A:ALA:HB1 | 4 | 0.15 | 0.02 | 0.15 |
| (1,3053) | 1:172:A:VAL:HG23 | 1:175:A:ALA:HB2 | 4 | 0.15 | 0.02 | 0.15 |
| (1,3053) | 1:172:A:VAL:HG23 | 1:175:A:ALA:HB3 | 4 | 0.15 | 0.02 | 0.15 |
| (1,184) | 1:60:A:HIS:H | 1:72:A:THR:HA | 4 | 0.14 | 0.04 | 0.12 |
| (1,2630) | 1:101:A:VAL:HG21 | 1:102:A:GLN:H | 4 | 0.14 | 0.01 | 0.14 |
| (1,2630) | 1:101:A:VAL:HG22 | 1:102:A:GLN:H | 4 | 0.14 | 0.01 | 0.14 |
| (1,2630) | 1:101:A:VAL:HG23 | 1:102:A:GLN:H | 4 | 0.14 | 0.01 | 0.14 |
| (1,3392) | 1:128:A:PHE:HA | 1:128:A:PHE:HD2 | 4 | 0.14 | 0.01 | 0.14 |
| (1,2519) | 1:127:A:SER:HA | 1:128:A:PHE:HB2 | 4 | 0.13 | 0.0 | 0.13 |
| (1,2787) | 1:86:A:LYS:H | 1:87:A:ILE:HG21 | 4 | 0.13 | 0.01 | 0.14 |
| (1,2787) | 1:86:A:LYS:H | 1:87:A:ILE:HG22 | 4 | 0.13 | 0.01 | 0.14 |
| (1,2787) | 1:86:A:LYS:H | 1:87:A:ILE:HG23 | 4 | 0.13 | 0.01 | 0.14 |
| (1,2226) | 1:111:A:PHE:HA | 1:116:A:VAL:HG11 | 4 | 0.12 | 0.03 | 0.11 |
| (1,2226) | 1:111:A:PHE:HA | 1:116:A:VAL:HG12 | 4 | 0.12 | 0.03 | 0.11 |
| (1,2226) | 1:111:A:PHE:HA | 1:116:A:VAL:HG13 | 4 | 0.12 | 0.03 | 0.11 |
| (1,2847) | 1:2:A:GLN:HA | 1:2:A:GLN:HB3 | 4 | 0.12 | 0.01 | 0.12 |
| (1,3531) | 1:58:A:LYS:H | 1:75:A:TRP:HZ2 | 4 | 0.12 | 0.02 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,126) | 1:10:A:ILE:HG21 | 1:159:A:GLN:H | 4 | 0.12 | 0.0 | 0.12 |
| (1,126) | 1:10:A:ILE:HG22 | 1:159:A:GLN:H | 4 | 0.12 | 0.0 | 0.12 |
| (1,126) | 1:10:A:ILE:HG23 | 1:159:A:GLN:H | 4 | 0.12 | 0.0 | 0.12 |
| (1,3527) | 1:73:A:GLN:HG2 | 1:125:A:TRP:HZ2 | 3 | 1.37 | 0.12 | 1.34 |
| (1,2339) | 1:186:A:GLU:HG3 | 1:187:A:LYS:HG2 | 3 | 1.27 | 0.75 | 1.68 |
| (1,3442) | 1:73:A:GLN:HG2 | 1:125:A:TRP:HH2 | 3 | 0.9 | 0.18 | 0.86 |
| (1,1444) | 1:83:A:VAL:HA | 1:85:A:ASP:HB2 | 3 | 0.7 | 0.23 | 0.75 |
| (1,3378) | 1:40:A:LEU:HD11 | 1:173:A:PHE:HD1 | 3 | 0.67 | 0.72 | 0.16 |
| (1,3378) | 1:40:A:LEU:HD11 | 1:173:A:PHE:HD2 | 3 | 0.67 | 0.72 | 0.16 |
| (1,3378) | 1:40:A:LEU:HD12 | 1:173:A:PHE:HD1 | 3 | 0.67 | 0.72 | 0.16 |
| (1,3378) | 1:40:A:LEU:HD12 | 1:173:A:PHE:HD2 | 3 | 0.67 | 0.72 | 0.16 |
| (1,3378) | 1:40:A:LEU:HD13 | 1:173:A:PHE:HD1 | 3 | 0.67 | 0.72 | 0.16 |
| (1,3378) | 1:40:A:LEU:HD13 | 1:173:A:PHE:HD2 | 3 | 0.67 | 0.72 | 0.16 |
| (1,1134) | 1:73:A:GLN:HE21 | 1:126:A:ASN:H | 3 | 0.49 | 0.06 | 0.53 |
| (1,1663) | 1:72:A:THR:HG21 | 1:138:A:GLU:HG3 | 3 | 0.47 | 0.31 | 0.39 |
| (1,1663) | 1:72:A:THR:HG22 | 1:138:A:GLU:HG3 | 3 | 0.47 | 0.31 | 0.39 |
| (1,1663) | 1:72:A:THR:HG23 | 1:138:A:GLU:HG3 | 3 | 0.47 | 0.31 | 0.39 |
| (1,979) | 1:29:A:TYR:H | 1:71:A:LEU:HD11 | 3 | 0.43 | 0.25 | 0.38 |
| (1,979) | 1:29:A:TYR:H | 1:71:A:LEU:HD12 | 3 | 0.43 | 0.25 | 0.38 |
| (1,979) | 1:29:A:TYR:H | 1:71:A:LEU:HD13 | 3 | 0.43 | 0.25 | 0.38 |
| (1,2195) | 1:66:A:PRO:HD2 | 1:67:A:LEU:HG | 3 | 0.34 | 0.1 | 0.39 |
| (1,1059) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HG3 | 3 | 0.32 | 0.17 | 0.2 |
| (1,118) | 1:159:A:GLN:H | 1:184:A:LEU:HD21 | 3 | 0.29 | 0.07 | 0.3 |
| (1,118) | 1:159:A:GLN:H | 1:184:A:LEU:HD22 | 3 | 0.29 | 0.07 | 0.3 |
| (1,118) | 1:159:A:GLN:H | 1:184:A:LEU:HD23 | 3 | 0.29 | 0.07 | 0.3 |
| (1,3345) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 3 | 0.28 | 0.08 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 3 | 0.28 | 0.08 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 3 | 0.28 | 0.08 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 3 | 0.28 | 0.08 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 3 | 0.28 | 0.08 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 3 | 0.28 | 0.08 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG21 | 1:177:A:TYR:HD1 | 3 | 0.28 | 0.08 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG21 | 1:177:A:TYR:HD2 | 3 | 0.28 | 0.08 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG22 | 1:177:A:TYR:HD1 | 3 | 0.28 | 0.08 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG22 | 1:177:A:TYR:HD2 | 3 | 0.28 | 0.08 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG23 | 1:177:A:TYR:HD1 | 3 | 0.28 | 0.08 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG23 | 1:177:A:TYR:HD2 | 3 | 0.28 | 0.08 | 0.33 |
| (1,1791) | 1:56:A:MET:HA | 1:56:A:MET:HG3 | 3 | 0.27 | 0.13 | 0.29 |
| (1,2699) | 1:134:A:VAL:HG11 | 1:138:A:GLU:HG3 | 3 | 0.27 | 0.08 | 0.28 |
| (1,2699) | 1:134:A:VAL:HG12 | 1:138:A:GLU:HG3 | 3 | 0.27 | 0.08 | 0.28 |
| (1,2699) | 1:134:A:VAL:HG13 | 1:138:A:GLU:HG3 | 3 | 0.27 | 0.08 | 0.28 |
| (1,2905) | 1:49:A:LYS:HA | 1:49:A:LYS:HD3 | 3 | 0.27 | 0.0 | 0.27 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,164) | 1:69:A:LYS:H | 1:69:A:LYS:HB3 | 3 | 0.26 | 0.06 | 0.3 |
| (1,2020) | 1:86:A:LYS:H | 1:86:A:LYS:HD2 | 3 | 0.25 | 0.05 | 0.28 |
| (1,3530) | 1:73:A:GLN:HE22 | 1:125:A:TRP:HZ2 | 3 | 0.24 | 0.08 | 0.29 |
| (1,1860) | 1:101:A:VAL:HB | 1:106:A:ASP:HB3 | 3 | 0.23 | 0.12 | 0.14 |
| (1,2832) | 1:55:A:LYS:HA | 1:56:A:MET:HB2 | 3 | 0.23 | 0.09 | 0.17 |
| (1,2479) | 1:8:A:GLN:HA | 1:8:A:GLN:HG2 | 3 | 0.21 | 0.08 | 0.23 |
| (1,2279) | 1:73:A:GLN:HG3 | 1:125:A:TRP:HA | 3 | 0.2 | 0.02 | 0.19 |
| (1,2220) | 1:67:A:LEU:HD11 | 1:103:A:SER:HB2 | 3 | 0.2 | 0.06 | 0.24 |
| (1,2220) | 1:67:A:LEU:HD12 | 1:103:A:SER:HB2 | 3 | 0.2 | 0.06 | 0.24 |
| (1,2220) | 1:67:A:LEU:HD13 | 1:103:A:SER:HB2 | 3 | 0.2 | 0.06 | 0.24 |
| (1,1703) | 1:59:A:TYR:HE1 | 1:136:A:GLN:HG3 | 3 | 0.19 | 0.06 | 0.21 |
| (1,1703) | 1:59:A:TYR:HE2 | 1:136:A:GLN:HG3 | 3 | 0.19 | 0.06 | 0.21 |
| (1,2347) | 1:131:A:LYS:HG3 | 1:131:A:LYS:HD2 | 3 | 0.19 | 0.0 | 0.19 |
| (1,2529) | 1:97:A:LYS:H | 1:98:A:THR:HG21 | 3 | 0.18 | 0.04 | 0.17 |
| (1,2529) | 1:97:A:LYS:H | 1:98:A:THR:HG22 | 3 | 0.18 | 0.04 | 0.17 |
| (1,2529) | 1:97:A:LYS:H | 1:98:A:THR:HG23 | 3 | 0.18 | 0.04 | 0.17 |
| (1,2274) | 1:4:A:THR:HA | 1:7:A:LYS:HB2 | 3 | 0.17 | 0.03 | 0.18 |
| (1,678) | 1:71:A:LEU:HD21 | 1:72:A:THR:H | 3 | 0.17 | 0.04 | 0.17 |
| (1,678) | 1:71:A:LEU:HD22 | 1:72:A:THR:H | 3 | 0.17 | 0.04 | 0.17 |
| (1,678) | 1:71:A:LEU:HD23 | 1:72:A:THR:H | 3 | 0.17 | 0.04 | 0.17 |
| (1,3430) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HB3 | 3 | 0.16 | 0.01 | 0.16 |
| (1,2766) | 1:39:A:VAL:HG21 | 1:40:A:LEU:H | 3 | 0.16 | 0.02 | 0.15 |
| (1,2766) | 1:39:A:VAL:HG22 | 1:40:A:LEU:H | 3 | 0.16 | 0.02 | 0.15 |
| (1,2766) | 1:39:A:VAL:HG23 | 1:40:A:LEU:H | 3 | 0.16 | 0.02 | 0.15 |
| (1,2417) | 1:73:A:GLN:HA | 1:77:A:VAL:HG21 | 3 | 0.14 | 0.02 | 0.15 |
| (1,2417) | 1:73:A:GLN:HA | 1:77:A:VAL:HG22 | 3 | 0.14 | 0.02 | 0.15 |
| (1,2417) | 1:73:A:GLN:HA | 1:77:A:VAL:HG23 | 3 | 0.14 | 0.02 | 0.15 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD11 | 3 | 0.14 | 0.03 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD12 | 3 | 0.14 | 0.03 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD13 | 3 | 0.14 | 0.03 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD21 | 3 | 0.14 | 0.03 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD22 | 3 | 0.14 | 0.03 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD23 | 3 | 0.14 | 0.03 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD11 | 3 | 0.14 | 0.03 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD12 | 3 | 0.14 | 0.03 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD13 | 3 | 0.14 | 0.03 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD21 | 3 | 0.14 | 0.03 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD22 | 3 | 0.14 | 0.03 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD23 | 3 | 0.14 | 0.03 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD11 | 3 | 0.14 | 0.03 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD12 | 3 | 0.14 | 0.03 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD13 | 3 | 0.14 | 0.03 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD21 | 3 | 0.14 | 0.03 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD22 | 3 | 0.14 | 0.03 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD23 | 3 | 0.14 | 0.03 | 0.14 |
| (1,3487) | 1:29:A:TYR:HE1 | 1:67:A:LEU:H | 3 | 0.14 | 0.02 | 0.13 |
| (1,3487) | 1:29:A:TYR:HE2 | 1:67:A:LEU:H | 3 | 0.14 | 0.02 | 0.13 |
| (1,2724) | 1:124:A:ALA:HA | 1:130:A:VAL:HG11 | 3 | 0.14 | 0.02 | 0.14 |
| (1,2724) | 1:124:A:ALA:HA | 1:130:A:VAL:HG12 | 3 | 0.14 | 0.02 | 0.14 |
| (1,2724) | 1:124:A:ALA:HA | 1:130:A:VAL:HG13 | 3 | 0.14 | 0.02 | 0.14 |
| (1,2596) | 1:63:A:PHE:HA | 1:64:A:LEU:H | 3 | 0.13 | 0.02 | 0.13 |
| (1,2657) | 1:167:A:THR:HA | 1:167:A:THR:HG21 | 3 | 0.13 | 0.01 | 0.14 |
| (1,2657) | 1:167:A:THR:HA | 1:167:A:THR:HG22 | 3 | 0.13 | 0.01 | 0.14 |
| (1,2657) | 1:167:A:THR:HA | 1:167:A:THR:HG23 | 3 | 0.13 | 0.01 | 0.14 |
| (1,3356) | 1:25:A:PHE:H | 1:25:A:PHE:HD1 | 3 | 0.13 | 0.02 | 0.14 |
| (1,3356) | 1:25:A:PHE:H | 1:25:A:PHE:HD2 | 3 | 0.13 | 0.02 | 0.14 |
| (1,1023) | 1:183:A:GLN:HG3 | 1:183:A:GLN:HE22 | 3 | 0.13 | 0.04 | 0.11 |
| (1,3212) | 1:87:A:ILE:HD11 | 1:91:A:MET:HG2 | 3 | 0.13 | 0.01 | 0.14 |
| (1,3212) | 1:87:A:ILE:HD11 | 1:91:A:MET:HG3 | 3 | 0.13 | 0.01 | 0.14 |
| (1,3212) | 1:87:A:ILE:HD12 | 1:91:A:MET:HG2 | 3 | 0.13 | 0.01 | 0.14 |
| (1,3212) | 1:87:A:ILE:HD12 | 1:91:A:MET:HG3 | 3 | 0.13 | 0.01 | 0.14 |
| (1,3212) | 1:87:A:ILE:HD13 | 1:91:A:MET:HG2 | 3 | 0.13 | 0.01 | 0.14 |
| (1,3212) | 1:87:A:ILE:HD13 | 1:91:A:MET:HG3 | 3 | 0.13 | 0.01 | 0.14 |
| (1,3371) | 1:167:A:THR:HG21 | 1:173:A:PHE:HD1 | 3 | 0.13 | 0.01 | 0.13 |
| (1,3371) | 1:167:A:THR:HG21 | 1:173:A:PHE:HD2 | 3 | 0.13 | 0.01 | 0.13 |
| (1,3371) | 1:167:A:THR:HG22 | 1:173:A:PHE:HD1 | 3 | 0.13 | 0.01 | 0.13 |
| (1,3371) | 1:167:A:THR:HG22 | 1:173:A:PHE:HD2 | 3 | 0.13 | 0.01 | 0.13 |
| (1,3371) | 1:167:A:THR:HG23 | 1:173:A:PHE:HD1 | 3 | 0.13 | 0.01 | 0.13 |
| (1,3371) | 1:167:A:THR:HG23 | 1:173:A:PHE:HD2 | 3 | 0.13 | 0.01 | 0.13 |
| (1,1431) | 1:85:A:ASP:HB3 | 1:87:A:ILE:H | 3 | 0.13 | 0.03 | 0.11 |
| (1,1676) | 1:163:A:GLN:H | 1:163:A:GLN:HG2 | 3 | 0.12 | 0.0 | 0.12 |
| (1,1676) | 1:163:A:GLN:H | 1:163:A:GLN:HG3 | 3 | 0.12 | 0.0 | 0.12 |
| (1,2115) | 1:10:A:ILE:H | 1:10:A:ILE:HG13 | 3 | 0.12 | 0.01 | 0.12 |
| (1,3402) | 1:26:A:PHE:H | 1:26:A:PHE:HD1 | 3 | 0.12 | 0.0 | 0.12 |
| (1,3402) | 1:26:A:PHE:H | 1:26:A:PHE:HD2 | 3 | 0.12 | 0.0 | 0.12 |
| (1,3521) | 1:162:A:PRO:HG2 | 1:177:A:TYR:HE1 | 3 | 0.12 | 0.02 | 0.12 |
| (1,3521) | 1:162:A:PRO:HG2 | 1:177:A:TYR:HE2 | 3 | 0.12 | 0.02 | 0.12 |
| (1,3521) | 1:162:A:PRO:HG3 | 1:177:A:TYR:HE1 | 3 | 0.12 | 0.02 | 0.12 |
| (1,3521) | 1:162:A:PRO:HG3 | 1:177:A:TYR:HE2 | 3 | 0.12 | 0.02 | 0.12 |
| (1,28) | 1:58:A:LYS:HG2 | 1:75:A:TRP:HE1 | 3 | 0.12 | 0.0 | 0.12 |
| (1,28) | 1:58:A:LYS:HG3 | 1:75:A:TRP:HE1 | 3 | 0.12 | 0.0 | 0.12 |
| (1,2890) | 1:71:A:LEU:HD21 | 1:74:A:ALA:HB1 | 3 | 0.12 | 0.01 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD21 | 1:74:A:ALA:HB2 | 3 | 0.12 | 0.01 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD21 | 1:74:A:ALA:HB3 | 3 | 0.12 | 0.01 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2890) | 1:71:A:LEU:HD22 | 1:74:A:ALA:HB1 | 3 | 0.12 | 0.01 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD22 | 1:74:A:ALA:HB2 | 3 | 0.12 | 0.01 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD22 | 1:74:A:ALA:HB3 | 3 | 0.12 | 0.01 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD23 | 1:74:A:ALA:HB1 | 3 | 0.12 | 0.01 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD23 | 1:74:A:ALA:HB2 | 3 | 0.12 | 0.01 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD23 | 1:74:A:ALA:HB3 | 3 | 0.12 | 0.01 | 0.11 |
| (1,3363) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HA | 3 | 0.12 | 0.0 | 0.12 |
| (1,3363) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HA | 3 | 0.12 | 0.0 | 0.12 |
| (1,985) | 1:93:A:GLU:HB2 | 1:95:A:VAL:H | 3 | 0.11 | 0.01 | 0.11 |
| (1,985) | 1:93:A:GLU:HB3 | 1:95:A:VAL:H | 3 | 0.11 | 0.01 | 0.11 |
| (1,2343) | 1:188:A:LYS:H | 1:188:A:LYS:HG2 | 3 | 0.11 | 0.01 | 0.12 |
| (1,2343) | 1:188:A:LYS:H | 1:188:A:LYS:HG3 | 3 | 0.11 | 0.01 | 0.12 |
| (1,238) | 1:74:A:ALA:H | 1:107:A:ILE:HG21 | 3 | 0.11 | 0.0 | 0.11 |
| (1,238) | 1:74:A:ALA:H | 1:107:A:ILE:HG22 | 3 | 0.11 | 0.0 | 0.11 |
| (1,238) | 1:74:A:ALA:H | 1:107:A:ILE:HG23 | 3 | 0.11 | 0.0 | 0.11 |
| (1,2742) | 1:77:A:VAL:HA | 1:130:A:VAL:HG11 | 3 | 0.11 | 0.01 | 0.11 |
| (1,2742) | 1:77:A:VAL:HA | 1:130:A:VAL:HG12 | 3 | 0.11 | 0.01 | 0.11 |
| (1,2742) | 1:77:A:VAL:HA | 1:130:A:VAL:HG13 | 3 | 0.11 | 0.01 | 0.11 |
| (1,223) | 1:40:A:LEU:HD11 | 1:170:A:MET:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,223) | 1:40:A:LEU:HD12 | 1:170:A:MET:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,223) | 1:40:A:LEU:HD13 | 1:170:A:MET:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,2879) | 1:59:A:TYR:HE1 | 1:140:A:ALA:HA | 3 | 0.11 | 0.01 | 0.1 |
| (1,2879) | 1:59:A:TYR:HE2 | 1:140:A:ALA:HA | 3 | 0.11 | 0.01 | 0.1 |
| (1,2996) | 1:140:A:ALA:HB1 | 1:141:A:ALA:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,2996) | 1:140:A:ALA:HB2 | 1:141:A:ALA:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,2996) | 1:140:A:ALA:HB3 | 1:141:A:ALA:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,3169) | 1:88:A:THR:H | 1:89:A:ALA:HB1 | 3 | 0.1 | 0.0 | 0.1 |
| (1,3169) | 1:88:A:THR:H | 1:89:A:ALA:HB2 | 3 | 0.1 | 0.0 | 0.1 |
| (1,3169) | 1:88:A:THR:H | 1:89:A:ALA:HB3 | 3 | 0.1 | 0.0 | 0.1 |
| (1,1709) | 1:87:A:ILE:HG21 | 1:88:A:THR:HA | 3 | 0.1 | 0.0 | 0.1 |
| (1,1709) | 1:87:A:ILE:HG22 | 1:88:A:THR:HA | 3 | 0.1 | 0.0 | 0.1 |
| (1,1709) | 1:87:A:ILE:HG23 | 1:88:A:THR:HA | 3 | 0.1 | 0.0 | 0.1 |
| (1,1990) | 1:133:A:LEU:HB3 | 1:136:A:GLN:HB2 | 2 | 1.05 | 0.17 | 1.05 |
| (1,2345) | 1:7:A:LYS:HG3 | 1:8:A:GLN:HB2 | 2 | 0.78 | 0.08 | 0.78 |
| (1,1573) | 1:119:A:GLU:HG2 | 1:120:A:ASP:HB2 | 2 | 0.7 | 0.35 | 0.7 |
| (1,904) | 1:127:A:SER:H | 1:127:A:SER:HB3 | 2 | 0.66 | 0.09 | 0.66 |
| (1,1283) | 1:64:A:LEU:HA | 1:65:A:GLY:HA3 | 2 | 0.64 | 0.03 | 0.64 |
| (1,1759) | 1:14:A:LYS:HB2 | 1:15:A:PRO:HA | 2 | 0.62 | 0.04 | 0.62 |
| (1,3412) | 1:36:A:PHE:HD1 | 1:40:A:LEU:HD11 | 2 | 0.6 | 0.46 | 0.6 |
| (1,3412) | 1:36:A:PHE:HD1 | 1:40:A:LEU:HD12 | 2 | 0.6 | 0.46 | 0.6 |
| (1,3412) | 1:36:A:PHE:HD1 | 1:40:A:LEU:HD13 | 2 | 0.6 | 0.46 | 0.6 |
| (1,3412) | 1:36:A:PHE:HD2 | 1:40:A:LEU:HD11 | 2 | 0.6 | 0.46 | 0.6 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3412) | 1:36:A:PHE:HD2 | 1:40:A:LEU:HD12 | 2 | 0.6 | 0.46 | 0.6 |
| (1,3412) | 1:36:A:PHE:HD2 | 1:40:A:LEU:HD13 | 2 | 0.6 | 0.46 | 0.6 |
| (1,1430) | 1:117:A:LYS:H | 1:120:A:ASP:HB2 | 2 | 0.45 | 0.04 | 0.45 |
| (1,2602) | 1:47:A:ARG:HG2 | 1:48:A:GLN:HA | 2 | 0.41 | 0.23 | 0.41 |
| (1,3494) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HG3 | 2 | 0.4 | 0.3 | 0.4 |
| (1,3494) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HG3 | 2 | 0.4 | 0.3 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG11 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG12 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG13 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG21 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG22 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG23 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG11 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG12 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG13 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG21 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG22 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG23 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG11 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG12 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG13 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG21 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG22 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG23 | 2 | 0.4 | 0.24 | 0.4 |
| (1,2334) | 1:3:A:ILE:HA | 1:8:A:GLN:HG3 | 2 | 0.35 | 0.21 | 0.35 |
| (1,1988) | 1:136:A:GLN:H | 1:136:A:GLN:HB2 | 2 | 0.31 | 0.02 | 0.31 |
| (1,1878) | 1:60:A:HIS:HB2 | 1:72:A:THR:HG21 | 2 | 0.3 | 0.18 | 0.3 |
| (1,1878) | 1:60:A:HIS:HB2 | 1:72:A:THR:HG22 | 2 | 0.3 | 0.18 | 0.3 |
| (1,1878) | 1:60:A:HIS:HB2 | 1:72:A:THR:HG23 | 2 | 0.3 | 0.18 | 0.3 |
| (1,1869) | 1:73:A:GLN:HG2 | 1:134:A:VAL:HG21 | 2 | 0.28 | 0.03 | 0.28 |
| (1,1869) | 1:73:A:GLN:HG2 | 1:134:A:VAL:HG22 | 2 | 0.28 | 0.03 | 0.28 |
| (1,1869) | 1:73:A:GLN:HG2 | 1:134:A:VAL:HG23 | 2 | 0.28 | 0.03 | 0.28 |
| (1,3287) | 1:30:A:CYS:HB3 | 1:31:A:PRO:HD3 | 2 | 0.24 | 0.03 | 0.24 |
| (1,2156) | 1:35:A:GLN:HG2 | 1:40:A:LEU:HG | 2 | 0.23 | 0.04 | 0.23 |
| (1,2156) | 1:35:A:GLN:HG3 | 1:40:A:LEU:HG | 2 | 0.23 | 0.04 | 0.23 |
| (1,3150) | 1:59:A:TYR:HA | 1:137:A:GLN:HG3 | 2 | 0.2 | 0.08 | 0.2 |
| (1,2535) | 1:20:A:PRO:HG2 | 1:57:A:THR:HG21 | 2 | 0.2 | 0.03 | 0.2 |
| (1,2535) | 1:20:A:PRO:HG2 | 1:57:A:THR:HG22 | 2 | 0.2 | 0.03 | 0.2 |
| (1,2535) | 1:20:A:PRO:HG2 | 1:57:A:THR:HG23 | 2 | 0.2 | 0.03 | 0.2 |
| (1,2535) | 1:20:A:PRO:HG3 | 1:57:A:THR:HG21 | 2 | 0.2 | 0.03 | 0.2 |
| (1,2535) | 1:20:A:PRO:HG3 | 1:57:A:THR:HG22 | 2 | 0.2 | 0.03 | 0.2 |
| (1,2535) | 1:20:A:PRO:HG3 | 1:57:A:THR:HG23 | 2 | 0.2 | 0.03 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2779) | 1:62:A:GLU:HA | 1:69:A:LYS:H | 2 | 0.2 | 0.03 | 0.2 |
| (1,1576) | 1:119:A:GLU:HG2 | 1:120:A:ASP:H | 2 | 0.2 | 0.09 | 0.2 |
| (1,1912) | 1:32:A:HIS:HB3 | 1:34:A:TYR:H | 2 | 0.18 | 0.0 | 0.18 |
| (1,1848) | 1:83:A:VAL:HB | 1:87:A:ILE:HG13 | 2 | 0.17 | 0.02 | 0.17 |
| (1,571) | 1:50:A:LEU:H | 1:50:A:LEU:HG | 2 | 0.16 | 0.06 | 0.16 |
| (1,1470) | 1:173:A:PHE:HB3 | 1:174:A:VAL:HG11 | 2 | 0.16 | 0.05 | 0.16 |
| (1,1470) | 1:173:A:PHE:HB3 | 1:174:A:VAL:HG12 | 2 | 0.16 | 0.05 | 0.16 |
| (1,1470) | 1:173:A:PHE:HB3 | 1:174:A:VAL:HG13 | 2 | 0.16 | 0.05 | 0.16 |
| (1,1989) | 1:136:A:GLN:HB2 | 1:137:A:GLN:H | 2 | 0.16 | 0.01 | 0.16 |
| (1,2214) | 1:120:A:ASP:HB2 | 1:121:A:TYR:HA | 2 | 0.16 | 0.03 | 0.16 |
| (1,1202) | 1:92:A:PHE:HD1 | 1:96:A:GLN:HE22 | 2 | 0.16 | 0.02 | 0.16 |
| (1,1202) | 1:92:A:PHE:HD2 | 1:96:A:GLN:HE22 | 2 | 0.16 | 0.02 | 0.16 |
| (1,3417) | 1:36:A:PHE:HD1 | 1:42:A:VAL:HG11 | 2 | 0.16 | 0.01 | 0.16 |
| (1,3417) | 1:36:A:PHE:HD1 | 1:42:A:VAL:HG12 | 2 | 0.16 | 0.01 | 0.16 |
| (1,3417) | 1:36:A:PHE:HD1 | 1:42:A:VAL:HG13 | 2 | 0.16 | 0.01 | 0.16 |
| (1,3417) | 1:36:A:PHE:HD2 | 1:42:A:VAL:HG11 | 2 | 0.16 | 0.01 | 0.16 |
| (1,3417) | 1:36:A:PHE:HD2 | 1:42:A:VAL:HG12 | 2 | 0.16 | 0.01 | 0.16 |
| (1,3417) | 1:36:A:PHE:HD2 | 1:42:A:VAL:HG13 | 2 | 0.16 | 0.01 | 0.16 |
| (1,570) | 1:50:A:LEU:H | 1:51:A:PRO:HD3 | 2 | 0.15 | 0.02 | 0.15 |
| (1,476) | 1:2:A:GLN:HB2 | 1:3:A:ILE:H | 2 | 0.14 | 0.0 | 0.14 |
| (1,3395) | 1:26:A:PHE:HD1 | 1:59:A:TYR:H | 2 | 0.14 | 0.02 | 0.14 |
| (1,3395) | 1:26:A:PHE:HD2 | 1:59:A:TYR:H | 2 | 0.14 | 0.02 | 0.14 |
| (1,3331) | 1:91:A:MET:H | 1:92:A:PHE:HD1 | 2 | 0.13 | 0.02 | 0.13 |
| (1,3331) | 1:91:A:MET:H | 1:92:A:PHE:HD2 | 2 | 0.13 | 0.02 | 0.13 |
| (1,3396) | 1:25:A:PHE:HA | 1:26:A:PHE:HD1 | 2 | 0.13 | 0.01 | 0.13 |
| (1,3396) | 1:25:A:PHE:HA | 1:26:A:PHE:HD2 | 2 | 0.13 | 0.01 | 0.13 |
| (1,747) | 1:118:A:GLY:HA2 | 1:119:A:GLU:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,3061) | 1:49:A:LYS:HB3 | 1:178:A:ALA:HB1 | 2 | 0.12 | 0.01 | 0.12 |
| (1,3061) | 1:49:A:LYS:HB3 | 1:178:A:ALA:HB2 | 2 | 0.12 | 0.01 | 0.12 |
| (1,3061) | 1:49:A:LYS:HB3 | 1:178:A:ALA:HB3 | 2 | 0.12 | 0.01 | 0.12 |
| (1,3436) | 1:75:A:TRP:HH2 | 1:87:A:ILE:HD11 | 2 | 0.12 | 0.01 | 0.12 |
| (1,3436) | 1:75:A:TRP:HH2 | 1:87:A:ILE:HD12 | 2 | 0.12 | 0.01 | 0.12 |
| (1,3436) | 1:75:A:TRP:HH2 | 1:87:A:ILE:HD13 | 2 | 0.12 | 0.01 | 0.12 |
| (1,3414) | 1:59:A:TYR:HD1 | 1:137:A:GLN:HB2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,3414) | 1:59:A:TYR:HD1 | 1:137:A:GLN:HB3 | 2 | 0.12 | 0.02 | 0.12 |
| (1,3414) | 1:59:A:TYR:HD2 | 1:137:A:GLN:HB2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,3414) | 1:59:A:TYR:HD2 | 1:137:A:GLN:HB3 | 2 | 0.12 | 0.02 | 0.12 |
| (1,2194) | 1:98:A:THR:HA | 1:98:A:THR:HG21 | 2 | 0.12 | 0.0 | 0.12 |
| (1,2194) | 1:98:A:THR:HA | 1:98:A:THR:HG22 | 2 | 0.12 | 0.0 | 0.12 |
| (1,2194) | 1:98:A:THR:HA | 1:98:A:THR:HG23 | 2 | 0.12 | 0.0 | 0.12 |
| (1,280) | 1:13:A:ASP:H | 1:14:A:LYS:HB2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,3286) | 1:81:A:LEU:HB2 | 1:82:A:GLY:HA3 | 2 | 0.12 | 0.02 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2176) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HD2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,2176) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HD3 | 2 | 0.12 | 0.0 | 0.12 |
| (1,2176) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HD2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,2176) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HD3 | 2 | 0.12 | 0.0 | 0.12 |
| (1,3132) | 1:24:A:GLU:HA | 1:152:A:MET:HE1 | 2 | 0.12 | 0.0 | 0.12 |
| (1,3132) | 1:24:A:GLU:HA | 1:152:A:MET:HE2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,3132) | 1:24:A:GLU:HA | 1:152:A:MET:HE3 | 2 | 0.12 | 0.0 | 0.12 |
| (1,3431) | 1:73:A:GLN:HE22 | 1:125:A:TRP:HD1 | 2 | 0.12 | 0.0 | 0.12 |
| (1,12) | 1:16:A:ILE:HD11 | 1:17:A:ALA:H | 2 | 0.11 | 0.01 | 0.11 |
| (1,12) | 1:16:A:ILE:HD12 | 1:17:A:ALA:H | 2 | 0.11 | 0.01 | 0.11 |
| (1,12) | 1:16:A:ILE:HD13 | 1:17:A:ALA:H | 2 | 0.11 | 0.01 | 0.11 |
| (1,91) | 1:187:A:LYS:H | 1:188:A:LYS:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,211) | 1:26:A:PHE:H | 1:151:A:ALA:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,795) | 1:176:A:GLN:HA | 1:179:A:ASP:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,1361) | 1:178:A:ALA:HB1 | 1:179:A:ASP:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1361) | 1:178:A:ALA:HB2 | 1:179:A:ASP:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1361) | 1:178:A:ALA:HB3 | 1:179:A:ASP:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2059) | 1:49:A:LYS:H | 1:49:A:LYS:HD2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2586) | 1:188:A:LYS:HA | 1:188:A:LYS:HG2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2586) | 1:188:A:LYS:HA | 1:188:A:LYS:HG3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2959) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HE1 | 2 | 0.11 | 0.01 | 0.11 |
| (1,2959) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HE2 | 2 | 0.11 | 0.01 | 0.11 |
| (1,2959) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HE1 | 2 | 0.11 | 0.01 | 0.11 |
| (1,2959) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HE2 | 2 | 0.11 | 0.01 | 0.11 |
| (1,2959) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HE1 | 2 | 0.11 | 0.01 | 0.11 |
| (1,2959) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HE2 | 2 | 0.11 | 0.01 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG2 | 1:178:A:ALA:HB1 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG2 | 1:178:A:ALA:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG2 | 1:178:A:ALA:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG3 | 1:178:A:ALA:HB1 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG3 | 1:178:A:ALA:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG3 | 1:178:A:ALA:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,335) | 1:165:A:MET:HE1 | 1:166:A:ASP:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,335) | 1:165:A:MET:HE2 | 1:166:A:ASP:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,335) | 1:165:A:MET:HE3 | 1:166:A:ASP:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,869) | 1:145:A:GLN:H | 1:146:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1223) | 1:161:A:ASN:HB2 | 1:164:A:GLY:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,1947) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HD2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1947) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HD3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2052) | 1:55:A:LYS:H | 1:55:A:LYS:HD2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2052) | 1:55:A:LYS:H | 1:55:A:LYS:HD3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2379) | 1:55:A:LYS:H | 1:55:A:LYS:HG2 | 2 | 0.11 | 0.0 | 0.11 |

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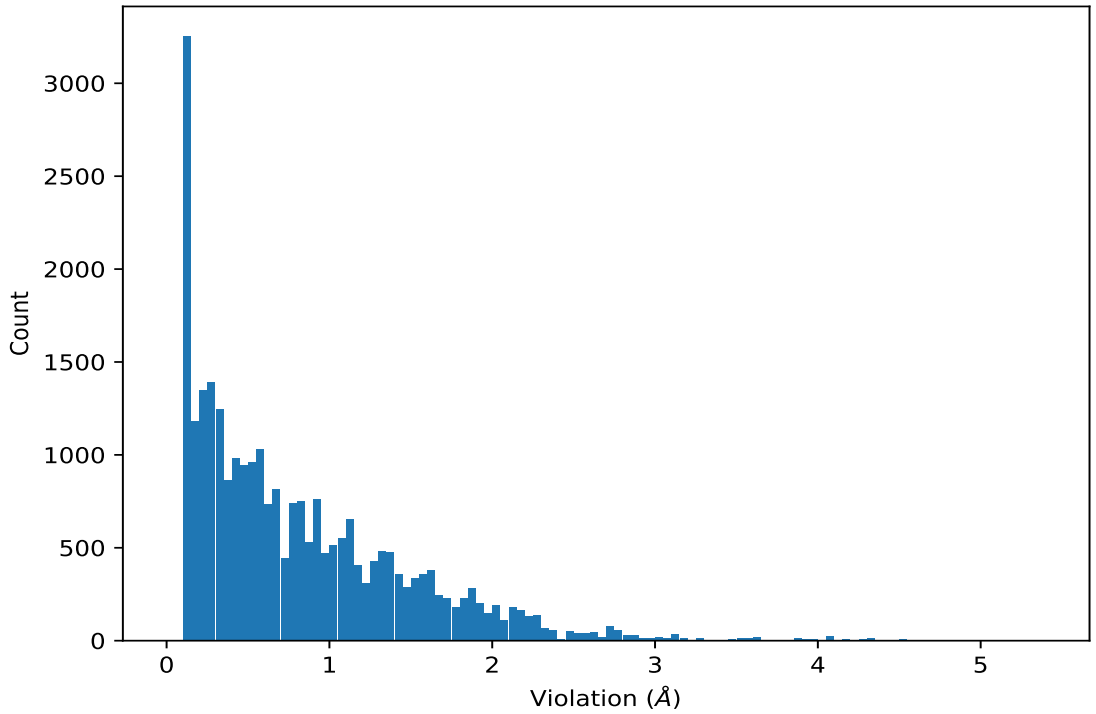
| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2379) | 1:55:A:LYS:H | 1:55:A:LYS:HG3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2653) | 1:38:A:GLU:HG2 | 1:88:A:THR:HG21 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2653) | 1:38:A:GLU:HG2 | 1:88:A:THR:HG22 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2653) | 1:38:A:GLU:HG2 | 1:88:A:THR:HG23 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2713) | 1:104:A:VAL:HG11 | 1:105:A:ALA:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,2713) | 1:104:A:VAL:HG12 | 1:105:A:ALA:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,2713) | 1:104:A:VAL:HG13 | 1:105:A:ALA:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,42) | 1:3:A:ILE:HD11 | 1:5:A:ASP:H | 2 | 0.1 | 0.0 | 0.1 |
| (1,42) | 1:3:A:ILE:HD12 | 1:5:A:ASP:H | 2 | 0.1 | 0.0 | 0.1 |
| (1,42) | 1:3:A:ILE:HD13 | 1:5:A:ASP:H | 2 | 0.1 | 0.0 | 0.1 |
| (1,930) | 1:183:A:GLN:H | 1:184:A:LEU:HG | 2 | 0.1 | 0.0 | 0.1 |
| (1,1264) | 1:29:A:TYR:HD1 | 1:64:A:LEU:HB3 | 2 | 0.1 | 0.0 | 0.1 |
| (1,1264) | 1:29:A:TYR:HD2 | 1:64:A:LEU:HB3 | 2 | 0.1 | 0.0 | 0.1 |
| (1,2296) | 1:24:A:GLU:H | 1:58:A:LYS:HG2 | 2 | 0.1 | 0.0 | 0.1 |
| (1,2296) | 1:24:A:GLU:H | 1:58:A:LYS:HG3 | 2 | 0.1 | 0.0 | 0.1 |
| (1,2803) | 1:73:A:GLN:HA | 1:76:A:ALA:HB1 | 2 | 0.1 | 0.0 | 0.1 |
| (1,2803) | 1:73:A:GLN:HA | 1:76:A:ALA:HB2 | 2 | 0.1 | 0.0 | 0.1 |
| (1,2803) | 1:73:A:GLN:HA | 1:76:A:ALA:HB3 | 2 | 0.1 | 0.0 | 0.1 |
| (1,3221) | 1:87:A:ILE:HD11 | 1:88:A:THR:HA | 2 | 0.1 | 0.0 | 0.1 |
| (1,3221) | 1:87:A:ILE:HD12 | 1:88:A:THR:HA | 2 | 0.1 | 0.0 | 0.1 |
| (1,3221) | 1:87:A:ILE:HD13 | 1:88:A:THR:HA | 2 | 0.1 | 0.0 | 0.1 |

[1]Number of violated models, [2]Standard deviation

## 9.5 All violated distance restraints (i)

### 9.5.1 Histogram : Distribution of distance violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.




### 9.5.2 Table : All distance violations (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 9 | 5.36 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 11 | 5.36 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 15 | 5.18 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 17 | 5.14 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 7 | 5.12 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 11 | 5.07 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 15 | 5.02 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 8 | 4.92 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 4 | 4.89 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 1 | 4.81 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 9 | 4.8 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 2 | 4.79 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 17 | 4.76 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 1 | 4.71 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 14 | 4.67 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 11 | 4.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 5 | 4.55 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 9 | 4.53 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 9 | 4.53 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 9 | 4.53 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 9 | 4.53 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 9 | 4.53 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 9 | 4.53 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 15 | 4.5 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 7 | 4.48 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 4 | 4.46 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 12 | 4.44 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 12 | 4.44 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 12 | 4.44 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 13 | 4.42 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 5 | 4.36 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 20 | 4.34 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 6 | 4.31 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 18 | 4.31 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 18 | 4.31 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 18 | 4.31 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 18 | 4.31 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 18 | 4.31 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 18 | 4.31 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 3 | 4.31 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 3 | 4.31 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 3 | 4.31 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 20 | 4.29 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 20 | 4.29 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 20 | 4.29 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 20 | 4.29 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 20 | 4.29 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 20 | 4.29 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 6 | 4.29 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 13 | 4.29 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 9 | 4.23 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 9 | 4.23 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 9 | 4.23 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 14 | 4.23 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 3 | 4.2 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 13 | 4.19 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 9 | 4.18 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 9 | 4.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 9 | 4.18 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 9 | 4.18 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 9 | 4.18 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 9 | 4.18 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 9 | 4.18 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 9 | 4.18 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 9 | 4.18 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 14 | 4.11 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 18 | 4.09 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 18 | 4.09 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 18 | 4.09 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 18 | 4.09 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 18 | 4.09 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 18 | 4.09 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 18 | 4.09 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 18 | 4.09 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 18 | 4.09 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 2 | 4.09 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 2 | 4.09 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 2 | 4.09 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 2 | 4.09 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 2 | 4.09 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 2 | 4.09 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 13 | 4.07 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 13 | 4.07 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 13 | 4.07 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 8 | 4.06 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 8 | 4.06 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 8 | 4.06 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 8 | 4.06 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 8 | 4.06 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 8 | 4.06 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 19 | 4.01 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 8 | 3.97 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 20 | 3.97 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 20 | 3.97 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 20 | 3.97 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 8 | 3.96 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 8 | 3.96 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 8 | 3.96 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 20 | 3.95 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 8 | 3.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 8 | 3.94 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 8 | 3.94 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 8 | 3.94 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 8 | 3.94 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 8 | 3.94 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 8 | 3.94 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 8 | 3.94 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 8 | 3.94 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 17 | 3.89 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 17 | 3.89 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 17 | 3.89 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 17 | 3.89 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 17 | 3.89 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 17 | 3.89 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 18 | 3.89 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 18 | 3.89 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 18 | 3.89 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 12 | 3.88 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 6 | 3.87 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 20 | 3.82 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 17 | 3.81 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 17 | 3.81 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 17 | 3.81 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 16 | 3.77 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 1 | 3.76 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 9 | 3.72 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 2 | 3.71 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 16 | 3.71 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 14 | 3.66 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 14 | 3.66 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 14 | 3.66 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 4 | 3.66 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 10 | 3.65 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 9 | 3.64 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 6 | 3.63 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 6 | 3.63 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 6 | 3.63 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 2 | 3.61 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 2 | 3.61 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 2 | 3.61 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 11 | 3.6 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 11 | 3.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 11 | 3.6 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 1 | 3.6 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 1 | 3.6 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 1 | 3.6 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 1 | 3.6 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 1 | 3.6 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 1 | 3.6 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 1 | 3.6 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 1 | 3.6 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 1 | 3.6 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 8 | 3.59 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 7 | 3.59 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 7 | 3.58 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 7 | 3.58 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 7 | 3.58 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 7 | 3.58 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 7 | 3.58 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 7 | 3.58 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 16 | 3.57 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 7 | 3.56 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 7 | 3.56 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 7 | 3.56 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 9 | 3.55 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 9 | 3.55 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 9 | 3.55 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 17 | 3.55 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 17 | 3.55 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 17 | 3.55 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 10 | 3.54 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 10 | 3.54 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 10 | 3.54 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 2 | 3.54 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 17 | 3.53 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 18 | 3.5 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 18 | 3.49 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 18 | 3.49 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 18 | 3.49 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 19 | 3.49 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 4 | 3.47 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 19 | 3.47 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 11 | 3.46 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 18 | 3.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 20 | 3.41 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 15 | 3.4 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 10 | 3.39 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 9 | 3.38 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 1 | 3.37 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 12 | 3.33 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 10 | 3.32 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 11 | 3.31 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 16 | 3.31 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 4 | 3.3 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 5 | 3.28 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 2 | 3.27 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 20 | 3.27 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 17 | 3.25 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 17 | 3.25 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 17 | 3.25 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 17 | 3.25 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 17 | 3.25 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 17 | 3.25 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 17 | 3.25 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 17 | 3.25 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 17 | 3.25 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 2 | 3.21 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 20 | 3.19 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 20 | 3.19 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 20 | 3.19 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 20 | 3.19 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 20 | 3.19 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 20 | 3.19 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 20 | 3.19 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 20 | 3.19 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 20 | 3.19 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 3 | 3.19 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 3 | 3.19 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 3 | 3.19 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 19 | 3.18 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 7 | 3.17 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 7 | 3.17 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 7 | 3.17 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 4 | 3.15 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 4 | 3.15 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 6 | 3.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 6 | 3.15 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 6 | 3.15 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 6 | 3.15 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 6 | 3.15 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 6 | 3.15 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 6 | 3.15 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 6 | 3.15 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 6 | 3.15 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 17 | 3.15 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 17 | 3.15 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 16 | 3.14 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 16 | 3.14 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 20 | 3.14 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 20 | 3.14 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 2 | 3.14 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 2 | 3.14 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 2 | 3.14 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 2 | 3.14 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 2 | 3.14 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 2 | 3.14 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 2 | 3.14 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 2 | 3.14 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 2 | 3.14 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 5 | 3.13 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 20 | 3.13 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 14 | 3.12 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 14 | 3.12 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 14 | 3.12 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 8 | 3.12 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 8 | 3.12 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 8 | 3.12 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 13 | 3.1 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 13 | 3.1 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 4 | 3.08 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 4 | 3.08 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 4 | 3.08 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 5 | 3.08 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 6 | 3.07 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 6 | 3.07 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 6 | 3.07 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 6 | 3.07 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 6 | 3.07 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 6 | 3.07 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 9 | 3.06 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 9 | 3.06 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 2 | 3.05 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 2 | 3.05 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 17 | 3.05 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 17 | 3.05 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 10 | 3.04 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 12 | 3.04 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 12 | 3.04 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 12 | 3.04 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 16 | 3.03 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 16 | 3.03 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 16 | 3.03 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 7 | 3.01 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 7 | 3.01 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 7 | 3.01 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 7 | 3.01 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 18 | 3.01 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 14 | 3.0 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 14 | 3.0 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 14 | 3.0 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 17 | 2.99 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 17 | 2.99 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 17 | 2.99 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 14 | 2.99 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 14 | 2.99 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 14 | 2.99 |
| (1,1772) | 1:11:A:THR:HB | 1:157:A:LYS:HG2 | 12 | 2.98 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 8 | 2.98 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 19 | 2.97 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 19 | 2.97 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 11 | 2.96 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 1 | 2.96 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 1 | 2.96 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 1 | 2.96 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 6 | 2.94 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 8 | 2.93 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 8 | 2.93 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 4 | 2.92 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 5 | 2.91 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 5 | 2.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 5 | 2.91 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 16 | 2.91 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 16 | 2.91 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 16 | 2.91 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 16 | 2.91 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 16 | 2.91 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 16 | 2.91 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 13 | 2.89 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 13 | 2.89 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 13 | 2.89 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 13 | 2.89 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 13 | 2.89 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 13 | 2.89 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 13 | 2.89 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 13 | 2.89 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 13 | 2.89 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 18 | 2.89 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 18 | 2.89 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 8 | 2.88 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 16 | 2.86 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 17 | 2.86 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 17 | 2.86 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 17 | 2.86 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 11 | 2.85 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 11 | 2.85 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 11 | 2.85 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 11 | 2.85 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 11 | 2.85 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 11 | 2.85 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 11 | 2.85 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 11 | 2.85 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 11 | 2.85 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 8 | 2.85 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 10 | 2.85 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 10 | 2.85 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 13 | 2.84 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 13 | 2.84 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 13 | 2.84 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 18 | 2.84 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 1 | 2.83 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 9 | 2.82 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 9 | 2.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 9 | 2.82 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 3 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 3 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 3 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 3 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 3 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 3 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 3 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 3 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 3 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 9 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 9 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 9 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 9 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 9 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 9 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 9 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 9 | 2.81 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 9 | 2.81 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 14 | 2.81 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 6 | 2.8 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 6 | 2.8 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 6 | 2.8 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 1 | 2.79 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 1 | 2.79 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 1 | 2.79 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 1 | 2.79 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 1 | 2.79 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 1 | 2.79 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 11 | 2.78 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 11 | 2.78 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 11 | 2.78 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 4 | 2.78 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 4 | 2.78 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 4 | 2.78 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 4 | 2.78 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 4 | 2.78 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 4 | 2.78 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 4 | 2.78 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 4 | 2.78 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 4 | 2.78 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 8 | 2.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 8 | 2.78 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 8 | 2.78 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 1 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 1 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 1 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 1 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 1 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 1 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 1 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 1 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 1 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 6 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 6 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 6 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 6 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 6 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 6 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 6 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 6 | 2.76 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 6 | 2.76 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 1 | 2.76 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 1 | 2.76 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 1 | 2.76 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 19 | 2.76 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 19 | 2.76 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 19 | 2.76 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 10 | 2.75 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 10 | 2.75 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 13 | 2.75 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 13 | 2.75 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 13 | 2.75 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 13 | 2.75 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 13 | 2.75 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 13 | 2.75 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 10 | 2.75 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 12 | 2.74 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 15 | 2.74 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 15 | 2.74 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 15 | 2.74 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 15 | 2.74 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 15 | 2.74 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 15 | 2.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 15 | 2.74 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 15 | 2.74 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 15 | 2.74 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 19 | 2.74 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 19 | 2.74 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 19 | 2.74 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 11 | 2.74 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 15 | 2.73 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 15 | 2.73 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 15 | 2.73 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 15 | 2.73 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 15 | 2.73 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 15 | 2.73 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 15 | 2.73 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 15 | 2.73 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 15 | 2.73 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 20 | 2.73 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 20 | 2.73 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 20 | 2.73 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 20 | 2.73 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 20 | 2.73 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 20 | 2.73 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 20 | 2.73 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 20 | 2.73 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 20 | 2.73 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 4 | 2.73 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 4 | 2.73 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 4 | 2.73 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 18 | 2.73 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 18 | 2.73 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 18 | 2.73 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 18 | 2.73 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 18 | 2.73 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 18 | 2.73 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 18 | 2.73 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 18 | 2.73 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 18 | 2.73 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 9 | 2.72 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 9 | 2.72 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 9 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 5 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 5 | 2.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 5 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 5 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 5 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 5 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 5 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 5 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 5 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 19 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 19 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 19 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 19 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 19 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 19 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 19 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 19 | 2.72 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 19 | 2.72 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 5 | 2.72 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 5 | 2.72 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 5 | 2.72 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 20 | 2.71 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 20 | 2.71 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 20 | 2.71 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 15 | 2.71 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 12 | 2.71 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 12 | 2.71 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 8 | 2.7 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 8 | 2.7 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 8 | 2.7 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 6 | 2.7 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 20 | 2.69 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 20 | 2.69 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 6 | 2.69 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 6 | 2.69 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 6 | 2.69 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 4 | 2.68 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 10 | 2.67 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 10 | 2.67 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 10 | 2.67 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 10 | 2.67 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 10 | 2.67 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 10 | 2.67 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 10 | 2.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 10 | 2.67 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 10 | 2.67 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 12 | 2.66 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 12 | 2.66 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 12 | 2.66 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 16 | 2.66 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 16 | 2.66 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 16 | 2.66 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 8 | 2.64 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 8 | 2.64 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 8 | 2.64 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 8 | 2.64 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 8 | 2.64 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 8 | 2.64 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 8 | 2.64 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 8 | 2.64 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 8 | 2.64 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 12 | 2.64 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 13 | 2.64 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 14 | 2.64 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 14 | 2.64 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 12 | 2.63 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 12 | 2.63 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 12 | 2.63 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 12 | 2.63 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 12 | 2.63 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 12 | 2.63 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 12 | 2.63 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 12 | 2.63 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 12 | 2.63 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 7 | 2.63 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 7 | 2.63 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 9 | 2.63 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 9 | 2.63 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 9 | 2.63 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 15 | 2.63 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 15 | 2.63 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 15 | 2.63 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 17 | 2.63 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 17 | 2.63 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 17 | 2.63 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 2 | 2.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 2 | 2.62 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 2 | 2.62 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 7 | 2.61 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 7 | 2.61 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 7 | 2.61 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 10 | 2.6 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 10 | 2.6 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 10 | 2.6 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 14 | 2.6 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 14 | 2.6 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 14 | 2.6 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 3 | 2.6 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 12 | 2.59 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 12 | 2.59 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 12 | 2.59 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 20 | 2.59 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 20 | 2.59 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 20 | 2.59 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 14 | 2.59 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 20 | 2.59 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 20 | 2.59 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 20 | 2.59 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 2 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 2 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 2 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 2 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 2 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 2 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 2 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 2 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 2 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 16 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 16 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 16 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 16 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 16 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 16 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 16 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 16 | 2.58 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 16 | 2.58 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 11 | 2.58 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 11 | 2.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 11 | 2.58 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 16 | 2.58 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 18 | 2.57 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 14 | 2.57 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 19 | 2.57 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 1 | 2.56 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 5 | 2.56 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 5 | 2.56 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 5 | 2.56 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 4 | 2.56 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 4 | 2.56 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 4 | 2.56 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 8 | 2.54 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 5 | 2.54 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 5 | 2.54 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 5 | 2.54 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 5 | 2.54 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 5 | 2.54 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 5 | 2.54 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 16 | 2.54 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 16 | 2.54 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 16 | 2.54 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 17 | 2.54 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 17 | 2.54 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 17 | 2.54 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 17 | 2.54 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 17 | 2.54 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 17 | 2.54 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 17 | 2.54 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 17 | 2.54 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 17 | 2.54 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 18 | 2.54 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 18 | 2.53 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 18 | 2.53 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 18 | 2.53 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 11 | 2.52 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 11 | 2.52 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 11 | 2.52 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 1 | 2.52 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 3 | 2.52 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 1 | 2.52 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 1 | 2.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 15 | 2.51 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 15 | 2.51 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 15 | 2.51 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 7 | 2.51 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 11 | 2.51 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 20 | 2.51 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 16 | 2.5 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 16 | 2.5 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 16 | 2.5 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 18 | 2.5 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 18 | 2.5 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 18 | 2.5 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 14 | 2.49 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 14 | 2.49 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 17 | 2.49 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 20 | 2.49 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 18 | 2.48 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 18 | 2.48 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 18 | 2.48 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 18 | 2.48 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 18 | 2.48 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 18 | 2.48 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 18 | 2.48 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 18 | 2.48 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 18 | 2.48 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 2 | 2.48 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 2 | 2.48 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 11 | 2.48 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 1 | 2.47 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 1 | 2.47 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 1 | 2.47 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 9 | 2.47 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 9 | 2.47 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 9 | 2.47 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 8 | 2.47 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 8 | 2.47 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 8 | 2.47 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 10 | 2.47 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 10 | 2.47 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 10 | 2.47 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 10 | 2.47 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 10 | 2.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 10 | 2.47 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 11 | 2.47 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 11 | 2.47 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 11 | 2.47 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 14 | 2.46 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 14 | 2.46 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 14 | 2.46 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 14 | 2.46 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 14 | 2.46 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 14 | 2.46 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 14 | 2.46 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 14 | 2.46 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 14 | 2.46 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 16 | 2.46 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 16 | 2.46 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 16 | 2.46 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 13 | 2.45 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 13 | 2.45 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 13 | 2.45 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 20 | 2.44 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 15 | 2.43 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 15 | 2.43 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 10 | 2.42 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 19 | 2.42 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 19 | 2.42 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 19 | 2.42 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 10 | 2.41 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 1 | 2.4 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 1 | 2.4 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 14 | 2.4 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 14 | 2.4 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 14 | 2.4 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 20 | 2.4 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 16 | 2.4 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 16 | 2.4 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 16 | 2.4 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 8 | 2.4 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 8 | 2.4 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 8 | 2.4 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 1 | 2.4 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 1 | 2.4 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 1 | 2.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 11 | 2.4 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 11 | 2.4 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 11 | 2.4 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 18 | 2.4 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 18 | 2.4 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 18 | 2.4 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 20 | 2.4 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 20 | 2.4 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 20 | 2.4 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 3 | 2.4 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 3 | 2.4 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 3 | 2.4 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 14 | 2.39 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 1 | 2.39 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 1 | 2.39 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 1 | 2.39 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 18 | 2.39 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 18 | 2.39 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 18 | 2.39 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 6 | 2.39 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 6 | 2.39 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 6 | 2.39 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 8 | 2.39 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 1 | 2.38 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 8 | 2.38 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 18 | 2.37 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 18 | 2.37 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 18 | 2.37 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 18 | 2.37 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 18 | 2.37 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 18 | 2.37 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 1 | 2.37 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 1 | 2.37 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 1 | 2.37 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 1 | 2.37 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 1 | 2.37 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 1 | 2.37 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 12 | 2.36 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 12 | 2.35 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 12 | 2.35 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 14 | 2.35 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 14 | 2.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 14 | 2.35 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 1 | 2.34 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 1 | 2.34 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 1 | 2.34 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 6 | 2.34 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 6 | 2.34 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 6 | 2.34 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 10 | 2.34 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 10 | 2.34 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 10 | 2.34 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 10 | 2.34 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 10 | 2.34 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 10 | 2.34 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 10 | 2.34 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 10 | 2.34 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 10 | 2.34 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 15 | 2.34 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 15 | 2.34 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 15 | 2.34 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 7 | 2.34 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 7 | 2.34 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 7 | 2.34 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 12 | 2.34 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 12 | 2.34 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 12 | 2.34 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 5 | 2.34 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 5 | 2.34 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 5 | 2.34 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 5 | 2.34 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 15 | 2.33 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 15 | 2.33 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 15 | 2.33 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 15 | 2.33 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 15 | 2.33 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 15 | 2.33 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 2 | 2.33 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 2 | 2.33 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 2 | 2.33 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 16 | 2.33 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 12 | 2.33 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 15 | 2.33 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 16 | 2.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 16 | 2.33 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 16 | 2.33 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 10 | 2.33 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 10 | 2.33 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 10 | 2.33 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 11 | 2.33 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 11 | 2.33 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 11 | 2.33 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 17 | 2.33 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 17 | 2.33 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 17 | 2.33 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 5 | 2.32 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 5 | 2.32 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 5 | 2.32 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 2 | 2.32 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 2 | 2.32 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 2 | 2.32 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 19 | 2.32 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 5 | 2.31 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 5 | 2.31 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 5 | 2.31 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 18 | 2.31 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 18 | 2.31 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 18 | 2.31 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 20 | 2.31 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 8 | 2.31 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 8 | 2.31 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 8 | 2.31 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 17 | 2.3 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 17 | 2.3 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 4 | 2.3 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 4 | 2.3 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 4 | 2.3 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 2 | 2.3 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 2 | 2.3 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 2 | 2.3 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 13 | 2.3 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 13 | 2.3 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 13 | 2.3 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 13 | 2.3 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 13 | 2.3 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 13 | 2.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 13 | 2.3 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 13 | 2.3 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 13 | 2.3 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 17 | 2.3 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 17 | 2.3 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 17 | 2.3 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 16 | 2.3 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 16 | 2.3 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 16 | 2.3 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 16 | 2.3 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 16 | 2.3 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 16 | 2.3 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 3 | 2.3 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 3 | 2.3 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 3 | 2.3 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 18 | 2.3 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 18 | 2.3 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 18 | 2.3 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 7 | 2.29 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 7 | 2.29 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 7 | 2.29 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 7 | 2.29 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 7 | 2.29 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 7 | 2.29 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 15 | 2.29 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 15 | 2.29 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 15 | 2.29 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 13 | 2.29 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 13 | 2.29 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 13 | 2.29 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 19 | 2.29 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 19 | 2.29 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 19 | 2.29 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 17 | 2.29 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 17 | 2.29 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 17 | 2.29 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 17 | 2.29 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 13 | 2.29 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 17 | 2.29 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 17 | 2.29 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 17 | 2.29 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 19 | 2.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 19 | 2.29 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 19 | 2.29 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 3 | 2.28 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 3 | 2.28 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 3 | 2.28 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 15 | 2.28 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 15 | 2.28 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 15 | 2.28 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 20 | 2.28 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 20 | 2.28 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 20 | 2.28 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 5 | 2.27 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 5 | 2.27 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 5 | 2.27 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 5 | 2.27 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 5 | 2.27 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 5 | 2.27 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 5 | 2.27 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 5 | 2.27 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 5 | 2.27 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 8 | 2.27 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 8 | 2.27 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 8 | 2.27 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 19 | 2.27 |
| (1,1351) | 1:179:A:ASP:HB2 | 1:183:A:GLN:HE21 | 17 | 2.27 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 7 | 2.26 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 7 | 2.26 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 7 | 2.26 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 7 | 2.26 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 7 | 2.26 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 7 | 2.26 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 14 | 2.26 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 14 | 2.26 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 14 | 2.26 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 4 | 2.26 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 4 | 2.26 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 4 | 2.26 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 4 | 2.26 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 4 | 2.26 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 4 | 2.26 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 14 | 2.26 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 16 | 2.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 16 | 2.26 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 16 | 2.26 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 13 | 2.25 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 13 | 2.25 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 13 | 2.25 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 16 | 2.25 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 16 | 2.25 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 16 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 4 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 4 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 4 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 4 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 4 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 4 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 4 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 4 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 4 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 19 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 19 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 19 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 19 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 19 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 19 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 19 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 19 | 2.25 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 19 | 2.25 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 17 | 2.25 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 5 | 2.25 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 5 | 2.25 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 5 | 2.25 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 20 | 2.25 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 20 | 2.25 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 20 | 2.25 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 13 | 2.25 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 17 | 2.25 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 3 | 2.25 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 3 | 2.25 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 3 | 2.25 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 14 | 2.25 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 14 | 2.25 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 14 | 2.25 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 11 | 2.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 11 | 2.24 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 16 | 2.24 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 16 | 2.24 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 10 | 2.24 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 10 | 2.24 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 10 | 2.24 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 10 | 2.24 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 10 | 2.24 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 10 | 2.24 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 7 | 2.24 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 10 | 2.24 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 2 | 2.24 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 8 | 2.24 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 8 | 2.24 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 8 | 2.24 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 8 | 2.24 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 8 | 2.24 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 8 | 2.24 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 10 | 2.24 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 10 | 2.24 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 10 | 2.24 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 16 | 2.23 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 16 | 2.23 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 16 | 2.23 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 11 | 2.23 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 11 | 2.23 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 11 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 16 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 16 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 16 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 16 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 16 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 16 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 16 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 16 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 16 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 20 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 20 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 20 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 20 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 20 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 20 | 2.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 20 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 20 | 2.23 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 20 | 2.23 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 2 | 2.23 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 2 | 2.23 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 2 | 2.23 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 9 | 2.23 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 18 | 2.23 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 18 | 2.23 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 18 | 2.23 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 18 | 2.23 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 18 | 2.23 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 18 | 2.23 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 1 | 2.23 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 1 | 2.23 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 1 | 2.23 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 2 | 2.22 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 2 | 2.22 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 2 | 2.22 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 17 | 2.22 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 17 | 2.22 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 17 | 2.22 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 6 | 2.22 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 15 | 2.22 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 15 | 2.22 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 15 | 2.22 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 11 | 2.22 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 11 | 2.22 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 11 | 2.22 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 12 | 2.22 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 12 | 2.22 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 12 | 2.22 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 11 | 2.21 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 11 | 2.21 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 11 | 2.21 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 11 | 2.21 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 11 | 2.21 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 11 | 2.21 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 2 | 2.21 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 2 | 2.21 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 16 | 2.21 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 16 | 2.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 16 | 2.21 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 16 | 2.21 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 16 | 2.21 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 16 | 2.21 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 19 | 2.21 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 19 | 2.21 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 19 | 2.21 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 19 | 2.21 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 19 | 2.21 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 19 | 2.21 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 5 | 2.21 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 5 | 2.21 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 5 | 2.21 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 12 | 2.21 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 12 | 2.21 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 12 | 2.21 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 17 | 2.21 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 17 | 2.21 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 17 | 2.21 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 15 | 2.21 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 15 | 2.21 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 15 | 2.21 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 7 | 2.21 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 3 | 2.21 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 3 | 2.21 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 3 | 2.21 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 1 | 2.2 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 1 | 2.2 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 1 | 2.2 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 1 | 2.2 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 1 | 2.2 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 1 | 2.2 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 1 | 2.2 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 1 | 2.2 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 1 | 2.2 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 17 | 2.2 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 17 | 2.2 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 17 | 2.2 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 9 | 2.2 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 9 | 2.2 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 9 | 2.2 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 10 | 2.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 10 | 2.2 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 10 | 2.2 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 5 | 2.2 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 5 | 2.2 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 5 | 2.2 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 6 | 2.2 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 16 | 2.2 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 8 | 2.19 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 8 | 2.19 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 8 | 2.19 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 4 | 2.19 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 4 | 2.19 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 4 | 2.19 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 7 | 2.19 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 7 | 2.19 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 7 | 2.19 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 8 | 2.19 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 8 | 2.19 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 8 | 2.19 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 8 | 2.19 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 8 | 2.19 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 8 | 2.19 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 8 | 2.19 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 8 | 2.19 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 8 | 2.19 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 17 | 2.19 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 17 | 2.19 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 17 | 2.19 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 19 | 2.19 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 19 | 2.19 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 19 | 2.19 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 17 | 2.19 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 17 | 2.19 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 17 | 2.19 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 10 | 2.19 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 10 | 2.19 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 10 | 2.19 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 6 | 2.19 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 20 | 2.19 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 20 | 2.19 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 20 | 2.19 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 16 | 2.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 16 | 2.19 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 16 | 2.19 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 14 | 2.18 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 14 | 2.18 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 14 | 2.18 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 14 | 2.18 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 14 | 2.18 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 14 | 2.18 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 7 | 2.18 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 7 | 2.18 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 7 | 2.18 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 8 | 2.18 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 8 | 2.18 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 8 | 2.18 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 2 | 2.18 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 2 | 2.18 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 2 | 2.18 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 2 | 2.18 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 2 | 2.18 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 2 | 2.18 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 2 | 2.18 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 2 | 2.18 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 2 | 2.18 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG11 | 7 | 2.18 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG12 | 7 | 2.18 |
| (1,2473) | 1:42:A:VAL:HG21 | 1:46:A:VAL:HG13 | 7 | 2.18 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG11 | 7 | 2.18 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG12 | 7 | 2.18 |
| (1,2473) | 1:42:A:VAL:HG22 | 1:46:A:VAL:HG13 | 7 | 2.18 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG11 | 7 | 2.18 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG12 | 7 | 2.18 |
| (1,2473) | 1:42:A:VAL:HG23 | 1:46:A:VAL:HG13 | 7 | 2.18 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 2 | 2.18 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 2 | 2.18 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 2 | 2.18 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 2 | 2.18 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 2 | 2.18 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 2 | 2.18 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 6 | 2.18 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 6 | 2.18 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 6 | 2.18 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 1 | 2.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 17 | 2.18 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 17 | 2.18 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 17 | 2.18 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 13 | 2.18 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 13 | 2.18 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 13 | 2.18 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 9 | 2.18 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 9 | 2.18 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 9 | 2.18 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 17 | 2.18 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 17 | 2.18 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 17 | 2.18 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 14 | 2.17 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 14 | 2.17 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 14 | 2.17 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 14 | 2.17 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 14 | 2.17 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 14 | 2.17 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 20 | 2.17 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 20 | 2.17 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 20 | 2.17 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 7 | 2.17 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 7 | 2.17 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 7 | 2.17 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 7 | 2.17 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 7 | 2.17 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 7 | 2.17 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 7 | 2.17 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 7 | 2.17 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 7 | 2.17 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 18 | 2.17 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 18 | 2.17 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 18 | 2.17 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 11 | 2.17 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 11 | 2.17 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 11 | 2.17 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 11 | 2.17 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 11 | 2.17 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 11 | 2.17 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 11 | 2.17 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 11 | 2.17 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 11 | 2.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 4 | 2.17 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 4 | 2.17 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 4 | 2.17 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 5 | 2.17 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 5 | 2.17 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 5 | 2.17 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 7 | 2.17 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 2 | 2.17 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 2 | 2.17 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 2 | 2.17 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 16 | 2.16 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 16 | 2.16 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 16 | 2.16 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 16 | 2.16 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 16 | 2.16 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 16 | 2.16 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 15 | 2.16 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 15 | 2.16 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 2 | 2.16 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 2 | 2.16 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 2 | 2.16 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 15 | 2.16 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 14 | 2.16 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 14 | 2.16 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 14 | 2.16 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 7 | 2.16 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 4 | 2.16 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 1 | 2.16 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 1 | 2.16 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 1 | 2.16 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 1 | 2.16 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 2 | 2.16 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 2 | 2.16 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 2 | 2.16 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 15 | 2.16 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 15 | 2.16 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 15 | 2.16 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 13 | 2.15 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 13 | 2.15 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 13 | 2.15 |
| (1,2370) | 1:12:A:LEU:H | 1:157:A:LYS:HG2 | 9 | 2.15 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 2 | 2.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 2 | 2.15 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 2 | 2.15 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 14 | 2.14 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 14 | 2.14 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 6 | 2.14 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 6 | 2.14 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 6 | 2.14 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 6 | 2.14 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 6 | 2.14 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 6 | 2.14 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 18 | 2.14 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 18 | 2.14 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 18 | 2.14 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 19 | 2.14 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 7 | 2.14 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 7 | 2.14 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 7 | 2.14 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 13 | 2.14 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 13 | 2.14 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 13 | 2.14 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 15 | 2.14 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 15 | 2.14 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 15 | 2.14 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 15 | 2.14 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 15 | 2.14 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 15 | 2.14 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 17 | 2.14 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 17 | 2.14 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 17 | 2.14 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 17 | 2.14 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 17 | 2.14 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 17 | 2.14 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 17 | 2.14 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 17 | 2.14 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 17 | 2.14 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 14 | 2.14 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 14 | 2.14 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 14 | 2.14 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 16 | 2.14 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 16 | 2.14 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 6 | 2.14 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 6 | 2.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 6 | 2.14 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 1 | 2.14 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 1 | 2.14 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 1 | 2.14 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 14 | 2.14 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 14 | 2.14 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 14 | 2.14 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 2 | 2.14 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 2 | 2.14 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 1 | 2.14 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 14 | 2.14 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 14 | 2.14 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 14 | 2.14 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 14 | 2.14 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 14 | 2.14 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 14 | 2.14 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 19 | 2.13 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 19 | 2.13 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 19 | 2.13 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE1 | 8 | 2.13 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE2 | 8 | 2.13 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE3 | 8 | 2.13 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 6 | 2.13 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 6 | 2.13 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 6 | 2.13 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 10 | 2.13 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 10 | 2.13 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 10 | 2.13 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 19 | 2.13 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 19 | 2.13 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 19 | 2.13 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 19 | 2.13 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 19 | 2.13 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 19 | 2.13 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 17 | 2.13 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 6 | 2.13 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 6 | 2.13 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 6 | 2.13 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 6 | 2.13 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 6 | 2.13 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 6 | 2.13 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 7 | 2.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 15 | 2.13 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 15 | 2.13 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 15 | 2.13 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 6 | 2.12 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 6 | 2.12 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 10 | 2.12 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 10 | 2.12 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 10 | 2.12 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 5 | 2.12 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 5 | 2.12 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 5 | 2.12 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE1 | 9 | 2.12 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE2 | 9 | 2.12 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE3 | 9 | 2.12 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 1 | 2.12 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 1 | 2.12 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 1 | 2.12 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 8 | 2.12 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 8 | 2.12 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 8 | 2.12 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 15 | 2.12 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 15 | 2.12 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 15 | 2.12 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 5 | 2.12 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 11 | 2.12 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 11 | 2.12 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 11 | 2.12 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 8 | 2.12 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 8 | 2.12 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 8 | 2.12 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 15 | 2.12 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 15 | 2.12 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 15 | 2.12 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 13 | 2.11 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 13 | 2.11 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 13 | 2.11 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 13 | 2.11 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 13 | 2.11 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 13 | 2.11 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 13 | 2.11 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 13 | 2.11 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 13 | 2.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 20 | 2.11 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 20 | 2.11 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 20 | 2.11 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 19 | 2.11 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 4 | 2.11 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 4 | 2.11 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 4 | 2.11 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 2 | 2.11 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 2 | 2.11 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 2 | 2.11 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 15 | 2.11 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 15 | 2.11 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 15 | 2.11 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 10 | 2.11 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 10 | 2.1 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 10 | 2.1 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 10 | 2.1 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 10 | 2.1 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 10 | 2.1 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 10 | 2.1 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 12 | 2.1 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 12 | 2.1 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 12 | 2.1 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 12 | 2.1 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 12 | 2.1 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 12 | 2.1 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 3 | 2.1 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 3 | 2.1 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 3 | 2.1 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 9 | 2.1 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 9 | 2.1 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 9 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 7 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 7 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 7 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 7 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 7 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 7 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 7 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 7 | 2.1 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 7 | 2.1 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 9 | 2.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 12 | 2.1 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 9 | 2.1 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 9 | 2.1 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 9 | 2.1 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 19 | 2.1 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 19 | 2.1 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 19 | 2.1 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 6 | 2.1 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 6 | 2.1 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 6 | 2.1 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 20 | 2.1 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 20 | 2.1 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 20 | 2.1 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 13 | 2.09 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 13 | 2.09 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 1 | 2.09 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 1 | 2.09 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 1 | 2.09 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 3 | 2.09 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 3 | 2.09 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 3 | 2.09 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 1 | 2.09 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 1 | 2.09 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 1 | 2.09 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 3 | 2.09 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 16 | 2.09 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 16 | 2.09 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 16 | 2.09 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 11 | 2.08 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 11 | 2.08 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 10 | 2.08 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 10 | 2.08 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 10 | 2.08 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 2 | 2.08 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 2 | 2.08 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 2 | 2.08 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 15 | 2.08 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 15 | 2.08 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 15 | 2.08 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 12 | 2.08 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 12 | 2.08 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 12 | 2.08 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 12 | 2.08 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 2 | 2.08 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 7 | 2.08 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 7 | 2.08 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 7 | 2.08 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 19 | 2.07 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 19 | 2.07 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 19 | 2.07 |
| (1,3293) | 1:16:A:ILE:HB | 1:156:A:GLY:HA2 | 3 | 2.07 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 12 | 2.07 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 12 | 2.07 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 12 | 2.07 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 12 | 2.07 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 12 | 2.07 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 12 | 2.07 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 12 | 2.07 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 12 | 2.07 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 12 | 2.07 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 14 | 2.07 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 14 | 2.07 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 14 | 2.07 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 14 | 2.07 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 14 | 2.07 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 14 | 2.07 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 7 | 2.07 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 7 | 2.07 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 7 | 2.07 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 1 | 2.07 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 1 | 2.07 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 1 | 2.07 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 18 | 2.07 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 13 | 2.07 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 13 | 2.07 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 13 | 2.07 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 8 | 2.07 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 13 | 2.07 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 4 | 2.07 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 4 | 2.07 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 4 | 2.07 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 18 | 2.07 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 18 | 2.07 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 18 | 2.07 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 6 | 2.07 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 6 | 2.07 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 6 | 2.07 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 1 | 2.06 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 1 | 2.06 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 11 | 2.06 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 11 | 2.06 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 11 | 2.06 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 11 | 2.06 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 11 | 2.06 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 11 | 2.06 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 2 | 2.06 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 2 | 2.06 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 2 | 2.06 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 2 | 2.06 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 2 | 2.06 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 2 | 2.06 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 5 | 2.06 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 5 | 2.06 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 5 | 2.06 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 5 | 2.06 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 5 | 2.06 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 5 | 2.06 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 5 | 2.06 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 5 | 2.06 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 5 | 2.06 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 18 | 2.06 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 18 | 2.06 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 18 | 2.06 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 1 | 2.06 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 1 | 2.06 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 1 | 2.06 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 17 | 2.06 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 17 | 2.06 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 17 | 2.06 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 15 | 2.06 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 19 | 2.06 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 19 | 2.06 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 19 | 2.06 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 2 | 2.06 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 2 | 2.06 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 2 | 2.06 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 3 | 2.05 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 3 | 2.05 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 4 | 2.05 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 4 | 2.05 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 19 | 2.05 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 19 | 2.05 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 19 | 2.05 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 19 | 2.05 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 19 | 2.05 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 19 | 2.05 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG11 | 20 | 2.05 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG12 | 20 | 2.05 |
| (1,2618) | 1:184:A:LEU:HB2 | 1:185:A:VAL:HG13 | 20 | 2.05 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 3 | 2.05 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 3 | 2.05 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 3 | 2.05 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 10 | 2.05 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 10 | 2.05 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 10 | 2.05 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 5 | 2.05 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 5 | 2.05 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 5 | 2.05 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 20 | 2.05 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 20 | 2.05 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 20 | 2.05 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 11 | 2.05 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 11 | 2.05 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 11 | 2.05 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 1 | 2.05 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 13 | 2.05 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 13 | 2.05 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 13 | 2.05 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 14 | 2.04 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 10 | 2.04 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 10 | 2.04 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 10 | 2.04 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 4 | 2.04 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 4 | 2.04 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 4 | 2.04 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 4 | 2.04 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 4 | 2.04 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 4 | 2.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 12 | 2.04 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 12 | 2.04 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 12 | 2.04 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 15 | 2.04 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 11 | 2.04 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 9 | 2.04 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 9 | 2.04 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 9 | 2.04 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 20 | 2.04 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 20 | 2.04 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 20 | 2.04 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 15 | 2.04 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 15 | 2.04 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 15 | 2.04 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 19 | 2.03 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 20 | 2.03 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 20 | 2.03 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 20 | 2.03 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 19 | 2.03 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 19 | 2.03 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 19 | 2.03 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 19 | 2.03 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 19 | 2.03 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 19 | 2.03 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 11 | 2.03 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 11 | 2.03 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 11 | 2.03 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 12 | 2.03 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 12 | 2.03 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 12 | 2.03 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 20 | 2.03 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 20 | 2.03 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 20 | 2.03 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 5 | 2.03 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 5 | 2.03 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 5 | 2.03 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 4 | 2.03 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 4 | 2.03 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 4 | 2.03 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 5 | 2.03 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 5 | 2.03 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 5 | 2.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 6 | 2.02 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 6 | 2.02 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 6 | 2.02 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 6 | 2.02 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 6 | 2.02 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 6 | 2.02 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 5 | 2.02 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 5 | 2.02 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 5 | 2.02 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 5 | 2.02 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 5 | 2.02 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 5 | 2.02 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 5 | 2.02 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 5 | 2.02 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 5 | 2.02 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 4 | 2.02 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 4 | 2.02 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 4 | 2.02 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 15 | 2.02 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 15 | 2.02 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 15 | 2.02 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 5 | 2.02 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 5 | 2.02 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 5 | 2.02 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 15 | 2.02 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 15 | 2.02 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 15 | 2.02 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 15 | 2.02 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 15 | 2.02 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 15 | 2.02 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 3 | 2.02 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 3 | 2.02 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 3 | 2.02 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 12 | 2.02 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 16 | 2.02 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 3 | 2.01 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 3 | 2.01 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 3 | 2.01 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 3 | 2.01 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 3 | 2.01 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 3 | 2.01 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 12 | 2.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 12 | 2.01 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 12 | 2.01 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 6 | 2.01 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 6 | 2.01 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 6 | 2.01 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 10 | 2.01 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 10 | 2.01 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 10 | 2.01 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 9 | 2.01 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 9 | 2.01 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 9 | 2.01 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 3 | 2.01 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 3 | 2.01 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 3 | 2.01 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 8 | 2.01 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 11 | 2.01 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 11 | 2.01 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 11 | 2.01 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 12 | 2.01 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 12 | 2.01 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 12 | 2.01 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 12 | 2.01 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 12 | 2.01 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 12 | 2.01 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 20 | 2.01 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 20 | 2.01 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 20 | 2.01 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 17 | 2.01 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 17 | 2.01 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 17 | 2.01 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 17 | 2.0 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 17 | 2.0 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 17 | 2.0 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 17 | 2.0 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 17 | 2.0 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 17 | 2.0 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 8 | 2.0 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 8 | 2.0 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 8 | 2.0 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 13 | 2.0 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 13 | 2.0 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 13 | 2.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 5 | 2.0 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 5 | 2.0 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 5 | 2.0 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 5 | 2.0 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 5 | 2.0 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 5 | 2.0 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 4 | 2.0 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 4 | 2.0 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 4 | 2.0 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 16 | 2.0 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 16 | 2.0 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 16 | 2.0 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 10 | 2.0 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 10 | 2.0 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 10 | 2.0 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 19 | 2.0 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 19 | 2.0 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 19 | 2.0 |
| (1,1351) | 1:179:A:ASP:HB2 | 1:183:A:GLN:HE21 | 9 | 2.0 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 10 | 2.0 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 10 | 2.0 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 10 | 2.0 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 8 | 2.0 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 8 | 2.0 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 8 | 2.0 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 7 | 1.99 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 7 | 1.99 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 7 | 1.99 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 7 | 1.99 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 7 | 1.99 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 7 | 1.99 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 2 | 1.99 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 2 | 1.99 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 2 | 1.99 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 10 | 1.99 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 1 | 1.99 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 1 | 1.99 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 1 | 1.99 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 18 | 1.99 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 16 | 1.99 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 16 | 1.99 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 16 | 1.99 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 8 | 1.99 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 8 | 1.99 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 10 | 1.99 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 1 | 1.99 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 1 | 1.99 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 1 | 1.99 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 5 | 1.99 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 5 | 1.99 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 5 | 1.99 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 14 | 1.99 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 14 | 1.99 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 14 | 1.99 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 15 | 1.99 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 15 | 1.99 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 15 | 1.99 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 9 | 1.98 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 9 | 1.98 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 9 | 1.98 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 9 | 1.98 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 9 | 1.98 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 9 | 1.98 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 1 | 1.98 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 1 | 1.98 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 1 | 1.98 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 2 | 1.98 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 2 | 1.98 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 2 | 1.98 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 5 | 1.98 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 5 | 1.98 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 10 | 1.98 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 10 | 1.98 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 10 | 1.98 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 11 | 1.98 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 11 | 1.98 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 11 | 1.98 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 19 | 1.98 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 8 | 1.97 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 8 | 1.97 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 8 | 1.97 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 8 | 1.97 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 8 | 1.97 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 8 | 1.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 13 | 1.97 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 13 | 1.97 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 13 | 1.97 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 12 | 1.97 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 12 | 1.97 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 12 | 1.97 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 2 | 1.97 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 2 | 1.97 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 2 | 1.97 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 12 | 1.97 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 12 | 1.97 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 12 | 1.97 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 7 | 1.97 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 7 | 1.97 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 7 | 1.97 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 13 | 1.97 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 13 | 1.97 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 13 | 1.97 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 13 | 1.97 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 13 | 1.97 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 13 | 1.97 |
| (1,1351) | 1:179:A:ASP:HB2 | 1:183:A:GLN:HE21 | 19 | 1.97 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 16 | 1.97 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 16 | 1.97 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 16 | 1.97 |
| (1,581) | 1:116:A:VAL:HG21 | 1:122:A:ASP:H | 7 | 1.97 |
| (1,581) | 1:116:A:VAL:HG22 | 1:122:A:ASP:H | 7 | 1.97 |
| (1,581) | 1:116:A:VAL:HG23 | 1:122:A:ASP:H | 7 | 1.97 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 3 | 1.97 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 3 | 1.97 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 3 | 1.97 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 7 | 1.97 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 7 | 1.97 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 7 | 1.97 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 6 | 1.96 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE1 | 18 | 1.96 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE2 | 18 | 1.96 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE3 | 18 | 1.96 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 9 | 1.96 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 9 | 1.96 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 9 | 1.96 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 9 | 1.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 9 | 1.96 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 9 | 1.96 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 9 | 1.96 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 9 | 1.96 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 9 | 1.96 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 15 | 1.96 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 15 | 1.96 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 15 | 1.96 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 8 | 1.96 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 8 | 1.96 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 8 | 1.96 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 17 | 1.96 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 17 | 1.96 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 17 | 1.96 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 17 | 1.96 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 17 | 1.96 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 17 | 1.96 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 17 | 1.96 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 17 | 1.96 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 17 | 1.96 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 20 | 1.96 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 20 | 1.96 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 20 | 1.96 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 20 | 1.96 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 20 | 1.96 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 20 | 1.96 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 6 | 1.96 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 6 | 1.96 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 6 | 1.96 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 5 | 1.96 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 5 | 1.96 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 5 | 1.96 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 6 | 1.96 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 6 | 1.96 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 6 | 1.96 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 5 | 1.96 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 5 | 1.96 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG21 | 17 | 1.96 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG22 | 17 | 1.96 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG23 | 17 | 1.96 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG21 | 17 | 1.96 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG22 | 17 | 1.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG23 | 17 | 1.96 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 8 | 1.96 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 8 | 1.96 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 8 | 1.96 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 15 | 1.95 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 15 | 1.95 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 19 | 1.95 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 19 | 1.95 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 8 | 1.95 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 8 | 1.95 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 8 | 1.95 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 9 | 1.95 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 9 | 1.95 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 9 | 1.95 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 5 | 1.95 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 13 | 1.95 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 13 | 1.95 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 13 | 1.95 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 13 | 1.95 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 13 | 1.95 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 13 | 1.95 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 9 | 1.95 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 9 | 1.95 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 9 | 1.95 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 13 | 1.95 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 13 | 1.95 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 13 | 1.95 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 20 | 1.95 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 20 | 1.95 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 20 | 1.95 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 14 | 1.95 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 14 | 1.95 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 14 | 1.95 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 1 | 1.95 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 1 | 1.95 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 1 | 1.95 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 5 | 1.94 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 5 | 1.94 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 5 | 1.94 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 18 | 1.94 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 18 | 1.94 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 18 | 1.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 19 | 1.94 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 19 | 1.94 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 19 | 1.94 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 19 | 1.94 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 19 | 1.94 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 19 | 1.94 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 19 | 1.94 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 19 | 1.94 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 19 | 1.94 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 19 | 1.94 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 19 | 1.94 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 19 | 1.94 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 19 | 1.94 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 19 | 1.94 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 19 | 1.94 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 19 | 1.94 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 19 | 1.94 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 19 | 1.94 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 11 | 1.94 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 11 | 1.94 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 11 | 1.94 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 11 | 1.94 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 11 | 1.94 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 11 | 1.94 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 11 | 1.94 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 11 | 1.94 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 11 | 1.94 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 19 | 1.94 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 19 | 1.94 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 19 | 1.94 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 19 | 1.94 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 19 | 1.94 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 19 | 1.94 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 3 | 1.94 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 3 | 1.94 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 3 | 1.94 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 18 | 1.94 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 18 | 1.94 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 18 | 1.94 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 2 | 1.94 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 2 | 1.94 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 2 | 1.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 4 | 1.94 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 4 | 1.94 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 4 | 1.94 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 9 | 1.94 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 9 | 1.94 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 9 | 1.94 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 12 | 1.94 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 12 | 1.94 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 12 | 1.94 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 7 | 1.94 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 7 | 1.94 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 7 | 1.94 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 6 | 1.94 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 5 | 1.93 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 5 | 1.93 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 20 | 1.93 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 20 | 1.93 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 5 | 1.93 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 5 | 1.93 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 5 | 1.93 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 5 | 1.93 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 5 | 1.93 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 5 | 1.93 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 1 | 1.93 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 1 | 1.93 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 1 | 1.93 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 9 | 1.93 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 9 | 1.93 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 9 | 1.93 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 10 | 1.93 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 10 | 1.93 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 10 | 1.93 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 17 | 1.93 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 17 | 1.93 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 17 | 1.93 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 18 | 1.93 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 18 | 1.93 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 18 | 1.93 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 14 | 1.93 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 14 | 1.93 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 14 | 1.93 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 7 | 1.93 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 7 | 1.93 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 7 | 1.93 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 19 | 1.93 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 19 | 1.93 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 19 | 1.93 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 15 | 1.93 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 15 | 1.93 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 15 | 1.93 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 9 | 1.92 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 9 | 1.92 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 3 | 1.92 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 3 | 1.92 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 3 | 1.92 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 3 | 1.92 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 3 | 1.92 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 3 | 1.92 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 12 | 1.92 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 12 | 1.92 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 12 | 1.92 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 16 | 1.92 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 16 | 1.92 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 16 | 1.92 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 19 | 1.92 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 19 | 1.92 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 19 | 1.92 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 8 | 1.92 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 8 | 1.92 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 8 | 1.92 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 16 | 1.92 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 16 | 1.92 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 16 | 1.92 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 3 | 1.92 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 3 | 1.92 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 15 | 1.92 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 15 | 1.92 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 6 | 1.92 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 18 | 1.92 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 18 | 1.92 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 18 | 1.92 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 13 | 1.92 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 13 | 1.92 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 13 | 1.92 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 16 | 1.92 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 16 | 1.92 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 16 | 1.92 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 6 | 1.91 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 6 | 1.91 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 8 | 1.91 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 8 | 1.91 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 2 | 1.91 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 2 | 1.91 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 2 | 1.91 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 2 | 1.91 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 10 | 1.91 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 1 | 1.91 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 17 | 1.91 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 1 | 1.91 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 1 | 1.91 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 1 | 1.91 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 5 | 1.91 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 5 | 1.91 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 5 | 1.91 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 6 | 1.91 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 6 | 1.91 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 6 | 1.91 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 20 | 1.91 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 20 | 1.91 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 20 | 1.91 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 17 | 1.91 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 17 | 1.91 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 17 | 1.91 |
| (1,2339) | 1:186:A:GLU:HG3 | 1:187:A:LYS:HG2 | 11 | 1.91 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 14 | 1.91 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 14 | 1.91 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 14 | 1.91 |
| (1,1351) | 1:179:A:ASP:HB2 | 1:183:A:GLN:HE21 | 12 | 1.91 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 7 | 1.91 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 7 | 1.91 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 7 | 1.91 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 4 | 1.91 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 4 | 1.91 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 4 | 1.91 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 12 | 1.9 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 12 | 1.9 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 12 | 1.9 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 12 | 1.9 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 12 | 1.9 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 12 | 1.9 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 13 | 1.9 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 13 | 1.9 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 13 | 1.9 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 13 | 1.9 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 13 | 1.9 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 13 | 1.9 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 15 | 1.9 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 15 | 1.9 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 15 | 1.9 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 17 | 1.9 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 17 | 1.9 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 17 | 1.9 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 17 | 1.9 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 17 | 1.9 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 17 | 1.9 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 17 | 1.9 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 17 | 1.9 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 17 | 1.9 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 6 | 1.9 |
| (1,2880) | 1:135:A:ALA:HA | 1:138:A:GLU:HB2 | 17 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 6 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 6 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 6 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 6 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 6 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 6 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 6 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 6 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 6 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 15 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 15 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 15 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 15 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 15 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 15 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 15 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 15 | 1.9 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 15 | 1.9 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 4 | 1.9 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 4 | 1.9 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 4 | 1.9 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 16 | 1.9 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 16 | 1.9 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 16 | 1.9 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 12 | 1.9 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 12 | 1.9 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 12 | 1.9 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 12 | 1.9 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 12 | 1.9 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 12 | 1.9 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 11 | 1.9 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 11 | 1.9 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 11 | 1.9 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 11 | 1.9 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 13 | 1.9 |
| (1,1351) | 1:179:A:ASP:HB2 | 1:183:A:GLN:HE21 | 10 | 1.9 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 20 | 1.9 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 20 | 1.9 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 20 | 1.9 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 10 | 1.89 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 10 | 1.89 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 10 | 1.89 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 10 | 1.89 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 10 | 1.89 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 10 | 1.89 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 14 | 1.89 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 14 | 1.89 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 14 | 1.89 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 16 | 1.89 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 16 | 1.89 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 16 | 1.89 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 3 | 1.89 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 3 | 1.89 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 3 | 1.89 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 9 | 1.89 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 9 | 1.89 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 9 | 1.89 |
| (1,1641) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HB | 3 | 1.89 |
| (1,1641) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HB | 3 | 1.89 |
| (1,1641) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HB | 3 | 1.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 4 | 1.89 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 3 | 1.89 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 3 | 1.89 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 3 | 1.89 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 4 | 1.89 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 4 | 1.89 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 4 | 1.89 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 11 | 1.89 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 11 | 1.89 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 11 | 1.89 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 6 | 1.89 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 6 | 1.89 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 6 | 1.89 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 14 | 1.89 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 14 | 1.89 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 14 | 1.89 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 3 | 1.88 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 3 | 1.88 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 3 | 1.88 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 17 | 1.88 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 17 | 1.88 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 17 | 1.88 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 17 | 1.88 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 17 | 1.88 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 17 | 1.88 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 14 | 1.88 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 14 | 1.88 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 14 | 1.88 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 14 | 1.88 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 14 | 1.88 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 14 | 1.88 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 14 | 1.88 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 14 | 1.88 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 14 | 1.88 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 3 | 1.88 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 3 | 1.88 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 3 | 1.88 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 19 | 1.88 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 19 | 1.88 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 19 | 1.88 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 16 | 1.88 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 16 | 1.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 16 | 1.88 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 16 | 1.88 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 16 | 1.88 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 16 | 1.88 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 16 | 1.88 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 16 | 1.88 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 16 | 1.88 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 17 | 1.88 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 17 | 1.88 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 17 | 1.88 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 4 | 1.88 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 4 | 1.88 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 4 | 1.88 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 18 | 1.88 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 18 | 1.88 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 18 | 1.88 |
| (1,1351) | 1:179:A:ASP:HB2 | 1:183:A:GLN:HE21 | 6 | 1.88 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 3 | 1.88 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 5 | 1.88 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 5 | 1.88 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 5 | 1.88 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 14 | 1.88 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 14 | 1.88 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 14 | 1.88 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 9 | 1.88 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 9 | 1.88 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 9 | 1.88 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 5 | 1.88 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 5 | 1.88 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 5 | 1.88 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 17 | 1.88 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 17 | 1.88 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 17 | 1.88 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 4 | 1.87 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 19 | 1.87 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 19 | 1.87 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 19 | 1.87 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 4 | 1.87 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 4 | 1.87 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 4 | 1.87 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 4 | 1.87 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 4 | 1.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 4 | 1.87 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 4 | 1.87 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 4 | 1.87 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 4 | 1.87 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 7 | 1.87 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 7 | 1.87 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 7 | 1.87 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 19 | 1.87 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 19 | 1.87 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 19 | 1.87 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 8 | 1.87 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 8 | 1.87 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 8 | 1.87 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 16 | 1.87 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 16 | 1.87 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 16 | 1.87 |
| (1,1351) | 1:179:A:ASP:HB2 | 1:183:A:GLN:HE21 | 3 | 1.87 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG11 | 13 | 1.87 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG12 | 13 | 1.87 |
| (1,947) | 1:40:A:LEU:H | 1:42:A:VAL:HG13 | 13 | 1.87 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 16 | 1.87 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 16 | 1.87 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 16 | 1.87 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 19 | 1.87 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 19 | 1.87 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 19 | 1.87 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 4 | 1.86 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 4 | 1.86 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 4 | 1.86 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 4 | 1.86 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 4 | 1.86 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 4 | 1.86 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 10 | 1.86 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 10 | 1.86 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 10 | 1.86 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 10 | 1.86 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 10 | 1.86 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 10 | 1.86 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 10 | 1.86 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 10 | 1.86 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 10 | 1.86 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 5 | 1.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 18 | 1.86 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 18 | 1.86 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 18 | 1.86 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 10 | 1.86 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 10 | 1.86 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 10 | 1.86 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 10 | 1.86 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 10 | 1.86 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 10 | 1.86 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 10 | 1.86 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 10 | 1.86 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 10 | 1.86 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 18 | 1.86 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 18 | 1.86 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 18 | 1.86 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 8 | 1.86 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 13 | 1.86 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 12 | 1.86 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 12 | 1.86 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 12 | 1.86 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 11 | 1.86 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 11 | 1.86 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 11 | 1.86 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG21 | 3 | 1.86 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG22 | 3 | 1.86 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG23 | 3 | 1.86 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG21 | 3 | 1.86 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG22 | 3 | 1.86 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG23 | 3 | 1.86 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 12 | 1.86 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 10 | 1.86 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 10 | 1.86 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 10 | 1.86 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 9 | 1.86 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 14 | 1.86 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 14 | 1.86 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 14 | 1.86 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 3 | 1.85 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 3 | 1.85 |
| (1,2880) | 1:135:A:ALA:HA | 1:138:A:GLU:HB2 | 2 | 1.85 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 4 | 1.85 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 4 | 1.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 4 | 1.85 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 7 | 1.85 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 7 | 1.85 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 7 | 1.85 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 2 | 1.85 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 2 | 1.85 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 2 | 1.85 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 5 | 1.85 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 5 | 1.85 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 5 | 1.85 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 2 | 1.85 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 2 | 1.85 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 2 | 1.85 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 17 | 1.85 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 17 | 1.85 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 10 | 1.85 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 10 | 1.85 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 10 | 1.85 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 6 | 1.85 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 6 | 1.85 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 11 | 1.85 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 11 | 1.85 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 11 | 1.85 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 7 | 1.85 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 7 | 1.85 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 7 | 1.85 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 16 | 1.85 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 16 | 1.85 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 16 | 1.85 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 1 | 1.84 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 1 | 1.84 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 1 | 1.84 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 1 | 1.84 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 1 | 1.84 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 1 | 1.84 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 18 | 1.84 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 18 | 1.84 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 18 | 1.84 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 18 | 1.84 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 18 | 1.84 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 18 | 1.84 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 20 | 1.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 20 | 1.84 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 20 | 1.84 |
| (1,2880) | 1:135:A:ALA:HA | 1:138:A:GLU:HB2 | 16 | 1.84 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 6 | 1.84 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 6 | 1.84 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 6 | 1.84 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 6 | 1.84 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 6 | 1.84 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 6 | 1.84 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 3 | 1.84 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 3 | 1.84 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 3 | 1.84 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 3 | 1.84 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 3 | 1.84 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 3 | 1.84 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 3 | 1.84 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 3 | 1.84 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 3 | 1.84 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 20 | 1.84 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 20 | 1.84 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 20 | 1.84 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 18 | 1.84 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 18 | 1.84 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 18 | 1.84 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 18 | 1.84 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 18 | 1.84 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 18 | 1.84 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 18 | 1.84 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 18 | 1.84 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 18 | 1.84 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 9 | 1.84 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 9 | 1.84 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 18 | 1.84 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 18 | 1.84 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 18 | 1.84 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 3 | 1.84 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 3 | 1.84 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 3 | 1.84 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 3 | 1.84 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 4 | 1.84 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 4 | 1.84 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 4 | 1.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 8 | 1.84 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 8 | 1.84 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 8 | 1.84 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG11 | 18 | 1.83 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG12 | 18 | 1.83 |
| (1,2580) | 1:94:A:ALA:HB1 | 1:95:A:VAL:HG13 | 18 | 1.83 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG11 | 18 | 1.83 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG12 | 18 | 1.83 |
| (1,2580) | 1:94:A:ALA:HB2 | 1:95:A:VAL:HG13 | 18 | 1.83 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG11 | 18 | 1.83 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG12 | 18 | 1.83 |
| (1,2580) | 1:94:A:ALA:HB3 | 1:95:A:VAL:HG13 | 18 | 1.83 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 7 | 1.83 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG21 | 5 | 1.83 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG22 | 5 | 1.83 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG23 | 5 | 1.83 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG21 | 5 | 1.83 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG22 | 5 | 1.83 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG23 | 5 | 1.83 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 1 | 1.83 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 1 | 1.83 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 1 | 1.83 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 13 | 1.83 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 13 | 1.83 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 13 | 1.83 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 2 | 1.83 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 2 | 1.83 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 2 | 1.83 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 10 | 1.83 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 10 | 1.83 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 10 | 1.83 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 16 | 1.82 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 16 | 1.82 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 16 | 1.82 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 16 | 1.82 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 16 | 1.82 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 16 | 1.82 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 16 | 1.82 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 16 | 1.82 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 16 | 1.82 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 20 | 1.82 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 20 | 1.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 20 | 1.82 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 20 | 1.82 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 20 | 1.82 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 20 | 1.82 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 20 | 1.82 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 20 | 1.82 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 20 | 1.82 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 2 | 1.82 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 2 | 1.82 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 2 | 1.82 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 2 | 1.82 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 2 | 1.82 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 2 | 1.82 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 7 | 1.82 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 7 | 1.82 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 7 | 1.82 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 17 | 1.82 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 17 | 1.82 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 17 | 1.82 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 17 | 1.82 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 17 | 1.82 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 17 | 1.82 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 17 | 1.82 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 17 | 1.82 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 17 | 1.82 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 8 | 1.82 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 8 | 1.82 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 8 | 1.82 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 2 | 1.82 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 2 | 1.82 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 2 | 1.82 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 7 | 1.82 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 7 | 1.82 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 7 | 1.82 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 13 | 1.82 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 13 | 1.82 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 13 | 1.82 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 20 | 1.81 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 20 | 1.81 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 20 | 1.81 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 20 | 1.81 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 20 | 1.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 20 | 1.81 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 20 | 1.81 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 20 | 1.81 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 20 | 1.81 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 12 | 1.81 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 12 | 1.81 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 12 | 1.81 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 12 | 1.81 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 12 | 1.81 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 12 | 1.81 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 12 | 1.81 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 12 | 1.81 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 12 | 1.81 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 15 | 1.81 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 15 | 1.81 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 15 | 1.81 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 13 | 1.81 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 13 | 1.81 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 13 | 1.81 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 13 | 1.81 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 13 | 1.81 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 13 | 1.81 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 13 | 1.81 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 13 | 1.81 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 13 | 1.81 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 8 | 1.81 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 8 | 1.81 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 8 | 1.81 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 8 | 1.81 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 8 | 1.81 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 8 | 1.81 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 5 | 1.81 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 11 | 1.81 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 11 | 1.81 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 11 | 1.81 |
| (1,1715) | 1:133:A:LEU:H | 1:136:A:GLN:HG2 | 5 | 1.81 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 7 | 1.81 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 7 | 1.81 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 7 | 1.81 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 4 | 1.81 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 6 | 1.81 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 6 | 1.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 6 | 1.81 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 15 | 1.8 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 15 | 1.8 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 15 | 1.8 |
| (1,3107) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HB2 | 17 | 1.8 |
| (1,3107) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HB2 | 17 | 1.8 |
| (1,3107) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HB2 | 17 | 1.8 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 11 | 1.8 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 1 | 1.8 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 1 | 1.8 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 1 | 1.8 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 1 | 1.8 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 1 | 1.8 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 1 | 1.8 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 1 | 1.8 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 1 | 1.8 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 1 | 1.8 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 14 | 1.8 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 14 | 1.8 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 14 | 1.8 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 15 | 1.8 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 15 | 1.8 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 15 | 1.8 |
| (1,2502) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HA | 10 | 1.8 |
| (1,2502) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HA | 10 | 1.8 |
| (1,2502) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HA | 10 | 1.8 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 3 | 1.8 |
| (1,1715) | 1:133:A:LEU:H | 1:136:A:GLN:HG2 | 4 | 1.8 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 3 | 1.8 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 3 | 1.8 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 3 | 1.8 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 9 | 1.8 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 9 | 1.8 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 9 | 1.8 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 10 | 1.8 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 10 | 1.8 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 10 | 1.8 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 8 | 1.8 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 8 | 1.8 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 8 | 1.8 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 3 | 1.8 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 3 | 1.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 3 | 1.8 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 18 | 1.8 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 18 | 1.8 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 18 | 1.8 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 14 | 1.79 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 15 | 1.79 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 19 | 1.79 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 19 | 1.79 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 19 | 1.79 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 19 | 1.79 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 19 | 1.79 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 19 | 1.79 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 19 | 1.79 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 19 | 1.79 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 19 | 1.79 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 4 | 1.79 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 9 | 1.79 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 9 | 1.79 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 9 | 1.79 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 18 | 1.79 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 18 | 1.79 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 18 | 1.79 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 18 | 1.79 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 18 | 1.79 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 18 | 1.79 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 4 | 1.79 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 4 | 1.79 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 4 | 1.79 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 17 | 1.79 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 8 | 1.79 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 8 | 1.79 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 8 | 1.79 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 8 | 1.79 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 8 | 1.79 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 8 | 1.79 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 8 | 1.79 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 8 | 1.79 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 8 | 1.79 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 1 | 1.79 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 1 | 1.79 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 1 | 1.79 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 15 | 1.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 15 | 1.79 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 3 | 1.79 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 3 | 1.79 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 3 | 1.79 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 4 | 1.79 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 19 | 1.79 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 19 | 1.79 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 19 | 1.79 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 17 | 1.78 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 16 | 1.78 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 16 | 1.78 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 16 | 1.78 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 4 | 1.78 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 4 | 1.78 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 4 | 1.78 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 7 | 1.78 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 7 | 1.78 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 7 | 1.78 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 11 | 1.78 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 11 | 1.78 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 11 | 1.78 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 6 | 1.78 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 6 | 1.78 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 6 | 1.78 |
| (1,1715) | 1:133:A:LEU:H | 1:136:A:GLN:HG2 | 16 | 1.78 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 13 | 1.78 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 13 | 1.78 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 13 | 1.78 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 13 | 1.78 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 13 | 1.78 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 13 | 1.78 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 2 | 1.78 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 2 | 1.78 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 2 | 1.78 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 15 | 1.78 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 15 | 1.78 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 15 | 1.78 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 12 | 1.78 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 12 | 1.78 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 12 | 1.78 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 20 | 1.78 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 20 | 1.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 20 | 1.78 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 14 | 1.77 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 3 | 1.77 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 3 | 1.77 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 3 | 1.77 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 20 | 1.77 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 20 | 1.77 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 20 | 1.77 |
| (1,1715) | 1:133:A:LEU:H | 1:136:A:GLN:HG2 | 20 | 1.77 |
| (1,1212) | 1:31:A:PRO:HG2 | 1:96:A:GLN:HE21 | 18 | 1.77 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 3 | 1.77 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 3 | 1.77 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 3 | 1.77 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 3 | 1.77 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 3 | 1.77 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 3 | 1.77 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 5 | 1.77 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 5 | 1.77 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 5 | 1.77 |
| (1,3107) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HB2 | 2 | 1.76 |
| (1,3107) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HB2 | 2 | 1.76 |
| (1,3107) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HB2 | 2 | 1.76 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 19 | 1.76 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 19 | 1.76 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 19 | 1.76 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 19 | 1.76 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 19 | 1.76 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 19 | 1.76 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 19 | 1.76 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 19 | 1.76 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 19 | 1.76 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 6 | 1.76 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 6 | 1.76 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 6 | 1.76 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 5 | 1.76 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 5 | 1.76 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 5 | 1.76 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 5 | 1.76 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 5 | 1.76 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 5 | 1.76 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 12 | 1.76 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 12 | 1.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 12 | 1.76 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 12 | 1.76 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 12 | 1.76 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 12 | 1.76 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 4 | 1.76 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 4 | 1.76 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 4 | 1.76 |
| (1,1545) | 1:186:A:GLU:HG3 | 1:187:A:LYS:HD3 | 14 | 1.76 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 5 | 1.76 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 18 | 1.76 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 3 | 1.75 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 3 | 1.75 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 3 | 1.75 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 3 | 1.75 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 3 | 1.75 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 3 | 1.75 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 3 | 1.75 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 3 | 1.75 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 3 | 1.75 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 3 | 1.75 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 6 | 1.75 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 6 | 1.75 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 6 | 1.75 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 8 | 1.75 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 8 | 1.75 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 8 | 1.75 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 15 | 1.75 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 15 | 1.75 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 15 | 1.75 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 15 | 1.75 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 15 | 1.75 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 15 | 1.75 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 5 | 1.75 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 5 | 1.75 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 5 | 1.75 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 8 | 1.75 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 8 | 1.75 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 8 | 1.75 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 16 | 1.75 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 16 | 1.75 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 16 | 1.75 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 16 | 1.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 4 | 1.75 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 4 | 1.75 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 4 | 1.75 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 6 | 1.75 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 6 | 1.75 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 6 | 1.75 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 9 | 1.75 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 9 | 1.75 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 9 | 1.75 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 19 | 1.75 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 19 | 1.75 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 19 | 1.75 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 16 | 1.75 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 16 | 1.75 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 16 | 1.75 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 15 | 1.75 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 2 | 1.74 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 2 | 1.74 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 2 | 1.74 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 2 | 1.74 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 2 | 1.74 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 2 | 1.74 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 10 | 1.74 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 10 | 1.74 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 20 | 1.74 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 20 | 1.74 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 20 | 1.74 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 20 | 1.74 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 20 | 1.74 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 20 | 1.74 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 13 | 1.74 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 13 | 1.74 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 13 | 1.74 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 13 | 1.74 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 13 | 1.74 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 13 | 1.74 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 13 | 1.74 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 13 | 1.74 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 13 | 1.74 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 1 | 1.74 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 1 | 1.74 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 1 | 1.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 1 | 1.74 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 1 | 1.74 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 1 | 1.74 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 1 | 1.74 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 1 | 1.74 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 1 | 1.74 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 6 | 1.74 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 6 | 1.74 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 6 | 1.74 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 13 | 1.74 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 13 | 1.74 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 13 | 1.74 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 7 | 1.74 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 7 | 1.74 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 7 | 1.74 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 15 | 1.74 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 15 | 1.74 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 15 | 1.74 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 15 | 1.74 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 15 | 1.74 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 15 | 1.74 |
| (1,2441) | 1:119:A:GLU:HA | 1:122:A:ASP:HB3 | 3 | 1.74 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 3 | 1.74 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 3 | 1.74 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 3 | 1.74 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 4 | 1.74 |
| (1,1715) | 1:133:A:LEU:H | 1:136:A:GLN:HG2 | 3 | 1.74 |
| (1,750) | 1:116:A:VAL:HG21 | 1:119:A:GLU:H | 11 | 1.74 |
| (1,750) | 1:116:A:VAL:HG22 | 1:119:A:GLU:H | 11 | 1.74 |
| (1,750) | 1:116:A:VAL:HG23 | 1:119:A:GLU:H | 11 | 1.74 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 18 | 1.74 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 18 | 1.74 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 18 | 1.74 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 11 | 1.74 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 11 | 1.74 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 11 | 1.74 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 7 | 1.74 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 7 | 1.74 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 7 | 1.74 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 2 | 1.74 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 20 | 1.73 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 20 | 1.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 20 | 1.73 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 20 | 1.73 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 20 | 1.73 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 20 | 1.73 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 13 | 1.73 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 13 | 1.73 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 13 | 1.73 |
| (1,3107) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HB2 | 16 | 1.73 |
| (1,3107) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HB2 | 16 | 1.73 |
| (1,3107) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HB2 | 16 | 1.73 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE1 | 17 | 1.73 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE2 | 17 | 1.73 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE3 | 17 | 1.73 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 6 | 1.73 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 6 | 1.73 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 6 | 1.73 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 6 | 1.73 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 6 | 1.73 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 6 | 1.73 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 6 | 1.73 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 6 | 1.73 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 6 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 2 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 2 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 2 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 2 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 2 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 2 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 2 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 2 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 2 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 16 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 16 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 16 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 16 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 16 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 16 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 16 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 16 | 1.73 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 16 | 1.73 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 14 | 1.73 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 14 | 1.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 14 | 1.73 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 14 | 1.73 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 14 | 1.73 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 14 | 1.73 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 12 | 1.73 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 12 | 1.73 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 12 | 1.73 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 18 | 1.73 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 18 | 1.73 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 18 | 1.73 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 10 | 1.72 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 10 | 1.72 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 10 | 1.72 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 10 | 1.72 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 10 | 1.72 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 10 | 1.72 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 12 | 1.72 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 12 | 1.72 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 12 | 1.72 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 12 | 1.72 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 12 | 1.72 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 12 | 1.72 |
| (1,2880) | 1:135:A:ALA:HA | 1:138:A:GLU:HB2 | 13 | 1.72 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 17 | 1.72 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 17 | 1.72 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 17 | 1.72 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 17 | 1.72 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 17 | 1.72 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 17 | 1.72 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG21 | 5 | 1.72 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG22 | 5 | 1.72 |
| (1,2394) | 1:131:A:LYS:HG3 | 1:134:A:VAL:HG23 | 5 | 1.72 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 3 | 1.72 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 3 | 1.72 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 3 | 1.72 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 15 | 1.72 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 1 | 1.72 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 1 | 1.72 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 1 | 1.72 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 18 | 1.72 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 18 | 1.72 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 18 | 1.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 10 | 1.72 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 5 | 1.72 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 5 | 1.72 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 5 | 1.72 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 12 | 1.72 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 12 | 1.72 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 12 | 1.72 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 12 | 1.72 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 12 | 1.72 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 12 | 1.72 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 17 | 1.72 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 17 | 1.72 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 17 | 1.72 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 20 | 1.72 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 20 | 1.72 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 20 | 1.72 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 15 | 1.72 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 15 | 1.72 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 15 | 1.72 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 3 | 1.72 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 3 | 1.72 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 3 | 1.72 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 10 | 1.72 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 10 | 1.72 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 10 | 1.72 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 3 | 1.72 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 3 | 1.72 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 3 | 1.72 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 15 | 1.71 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 15 | 1.71 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 15 | 1.71 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 15 | 1.71 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 15 | 1.71 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 15 | 1.71 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 9 | 1.71 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 9 | 1.71 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 9 | 1.71 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 9 | 1.71 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 9 | 1.71 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 9 | 1.71 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 9 | 1.71 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 9 | 1.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 9 | 1.71 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 7 | 1.71 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 7 | 1.71 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 7 | 1.71 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 7 | 1.71 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 7 | 1.71 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 7 | 1.71 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 7 | 1.71 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 7 | 1.71 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 7 | 1.71 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 5 | 1.71 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 5 | 1.71 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 5 | 1.71 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 19 | 1.71 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 19 | 1.71 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 19 | 1.71 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 5 | 1.71 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 5 | 1.71 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 5 | 1.71 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 12 | 1.71 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 12 | 1.71 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 12 | 1.71 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 3 | 1.71 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 3 | 1.71 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 3 | 1.71 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 16 | 1.71 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 16 | 1.71 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 16 | 1.71 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 11 | 1.71 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 11 | 1.71 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 11 | 1.71 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 4 | 1.71 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 4 | 1.71 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 4 | 1.71 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 13 | 1.71 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 13 | 1.71 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 13 | 1.71 |
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 5 | 1.7 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 8 | 1.7 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 8 | 1.7 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 8 | 1.7 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 13 | 1.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 13 | 1.7 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 13 | 1.7 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 11 | 1.7 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 11 | 1.7 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 11 | 1.7 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 11 | 1.7 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 11 | 1.7 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 11 | 1.7 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 11 | 1.7 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 11 | 1.7 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 11 | 1.7 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 9 | 1.7 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 14 | 1.7 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 1 | 1.7 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 19 | 1.7 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 19 | 1.7 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 19 | 1.7 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 20 | 1.7 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 20 | 1.7 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 20 | 1.7 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 18 | 1.7 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 6 | 1.7 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 6 | 1.7 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 6 | 1.7 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 5 | 1.7 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 5 | 1.7 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 5 | 1.7 |
| (1,402) | 1:116:A:VAL:HG21 | 1:120:A:ASP:H | 1 | 1.7 |
| (1,402) | 1:116:A:VAL:HG22 | 1:120:A:ASP:H | 1 | 1.7 |
| (1,402) | 1:116:A:VAL:HG23 | 1:120:A:ASP:H | 1 | 1.7 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 10 | 1.7 |
| (1,3378) | 1:40:A:LEU:HD11 | 1:173:A:PHE:HD1 | 18 | 1.69 |
| (1,3378) | 1:40:A:LEU:HD11 | 1:173:A:PHE:HD2 | 18 | 1.69 |
| (1,3378) | 1:40:A:LEU:HD12 | 1:173:A:PHE:HD1 | 18 | 1.69 |
| (1,3378) | 1:40:A:LEU:HD12 | 1:173:A:PHE:HD2 | 18 | 1.69 |
| (1,3378) | 1:40:A:LEU:HD13 | 1:173:A:PHE:HD1 | 18 | 1.69 |
| (1,3378) | 1:40:A:LEU:HD13 | 1:173:A:PHE:HD2 | 18 | 1.69 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 3 | 1.69 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 3 | 1.69 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 3 | 1.69 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 3 | 1.69 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 3 | 1.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 3 | 1.69 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 3 | 1.69 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 3 | 1.69 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 3 | 1.69 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 9 | 1.69 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 17 | 1.69 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 17 | 1.69 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 17 | 1.69 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 17 | 1.69 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 17 | 1.69 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 17 | 1.69 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 17 | 1.69 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 17 | 1.69 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 17 | 1.69 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 13 | 1.69 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 13 | 1.69 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 13 | 1.69 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 9 | 1.69 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 9 | 1.69 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 9 | 1.69 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 17 | 1.69 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 17 | 1.69 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 17 | 1.69 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 2 | 1.69 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 15 | 1.69 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 15 | 1.69 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 15 | 1.69 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 15 | 1.69 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 15 | 1.69 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 15 | 1.69 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 15 | 1.69 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 15 | 1.69 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 15 | 1.69 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 18 | 1.69 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 18 | 1.69 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 18 | 1.69 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 16 | 1.69 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 16 | 1.69 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 16 | 1.69 |
| (1,1427) | 1:143:A:ASP:HB2 | 1:145:A:GLN:HE22 | 1 | 1.69 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 1 | 1.69 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 1 | 1.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 1 | 1.69 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 11 | 1.69 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 5 | 1.69 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 9 | 1.69 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 9 | 1.69 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 9 | 1.69 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 9 | 1.68 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 9 | 1.68 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 9 | 1.68 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 9 | 1.68 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 9 | 1.68 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 9 | 1.68 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 18 | 1.68 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 18 | 1.68 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 1 | 1.68 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 1 | 1.68 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 1 | 1.68 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 14 | 1.68 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 14 | 1.68 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 14 | 1.68 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 14 | 1.68 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 14 | 1.68 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 14 | 1.68 |
| (1,2339) | 1:186:A:GLU:HG3 | 1:187:A:LYS:HG2 | 14 | 1.68 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 4 | 1.68 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 4 | 1.68 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 4 | 1.68 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 11 | 1.68 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 11 | 1.68 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 11 | 1.68 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 11 | 1.68 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 17 | 1.68 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 17 | 1.68 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 17 | 1.68 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 13 | 1.68 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 13 | 1.68 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 13 | 1.68 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 3 | 1.68 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 3 | 1.68 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 3 | 1.68 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 15 | 1.67 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 15 | 1.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 15 | 1.67 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 15 | 1.67 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 15 | 1.67 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 15 | 1.67 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 19 | 1.67 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 19 | 1.67 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 19 | 1.67 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 11 | 1.67 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 11 | 1.67 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 11 | 1.67 |
| (1,2880) | 1:135:A:ALA:HA | 1:138:A:GLU:HB2 | 15 | 1.67 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 1 | 1.67 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 1 | 1.67 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 1 | 1.67 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 16 | 1.67 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 16 | 1.67 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 16 | 1.67 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 16 | 1.67 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 16 | 1.67 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 16 | 1.67 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 17 | 1.67 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 17 | 1.67 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 17 | 1.67 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 17 | 1.67 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 17 | 1.67 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 17 | 1.67 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 17 | 1.67 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 17 | 1.67 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 17 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 7 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 7 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 7 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 7 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 7 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 7 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 7 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 7 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 7 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 14 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 14 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 14 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 14 | 1.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 14 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 14 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 14 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 14 | 1.67 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 14 | 1.67 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 6 | 1.67 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 6 | 1.67 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 2 | 1.67 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 2 | 1.67 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 2 | 1.67 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 13 | 1.67 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 12 | 1.67 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 12 | 1.67 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 12 | 1.67 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 4 | 1.67 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 4 | 1.67 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 4 | 1.67 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 5 | 1.67 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 5 | 1.67 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 5 | 1.67 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 15 | 1.67 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 15 | 1.67 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 15 | 1.67 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 18 | 1.66 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 18 | 1.66 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 18 | 1.66 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 18 | 1.66 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 18 | 1.66 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 18 | 1.66 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 16 | 1.66 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 16 | 1.66 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 16 | 1.66 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 16 | 1.66 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 16 | 1.66 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 16 | 1.66 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 13 | 1.66 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 13 | 1.66 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 6 | 1.66 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 6 | 1.66 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 6 | 1.66 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 13 | 1.66 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 13 | 1.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 13 | 1.66 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 8 | 1.66 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 8 | 1.66 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 8 | 1.66 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 7 | 1.66 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 11 | 1.66 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 9 | 1.66 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 9 | 1.66 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 9 | 1.66 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 13 | 1.66 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 13 | 1.66 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 13 | 1.66 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 6 | 1.66 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 6 | 1.66 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 6 | 1.66 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 5 | 1.66 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 5 | 1.66 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 5 | 1.66 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 13 | 1.66 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 13 | 1.66 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 17 | 1.66 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 17 | 1.66 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 17 | 1.66 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 17 | 1.66 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 1 | 1.66 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 11 | 1.66 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 7 | 1.66 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 7 | 1.66 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 7 | 1.66 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 14 | 1.66 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 14 | 1.66 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 14 | 1.66 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 18 | 1.65 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 18 | 1.65 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 18 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 3 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 3 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 3 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 5 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 5 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 5 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 9 | 1.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 9 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 9 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 12 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 12 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 12 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 15 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 15 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 15 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 16 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 16 | 1.65 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 16 | 1.65 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 11 | 1.65 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 11 | 1.65 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 11 | 1.65 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 8 | 1.65 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 8 | 1.65 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 8 | 1.65 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 8 | 1.65 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 8 | 1.65 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 8 | 1.65 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 8 | 1.65 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 8 | 1.65 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 8 | 1.65 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 20 | 1.65 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 20 | 1.65 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 20 | 1.65 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 6 | 1.65 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 6 | 1.65 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 6 | 1.65 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 4 | 1.65 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 4 | 1.65 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 4 | 1.65 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 7 | 1.65 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 7 | 1.65 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 7 | 1.65 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 10 | 1.65 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 10 | 1.65 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 10 | 1.65 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 9 | 1.65 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 9 | 1.65 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 9 | 1.65 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 9 | 1.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 9 | 1.65 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 9 | 1.65 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 9 | 1.65 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 9 | 1.65 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 9 | 1.65 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 2 | 1.65 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 2 | 1.65 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 2 | 1.65 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 19 | 1.65 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 20 | 1.65 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 20 | 1.65 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 20 | 1.65 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 4 | 1.65 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 4 | 1.65 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 4 | 1.65 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 8 | 1.65 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 8 | 1.65 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 8 | 1.65 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 9 | 1.65 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 9 | 1.65 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 9 | 1.65 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG21 | 12 | 1.65 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG22 | 12 | 1.65 |
| (1,1396) | 1:166:A:ASP:HB2 | 1:172:A:VAL:HG23 | 12 | 1.65 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 9 | 1.65 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 9 | 1.65 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 9 | 1.65 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 14 | 1.65 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 14 | 1.65 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 14 | 1.65 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 15 | 1.65 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 15 | 1.65 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 15 | 1.65 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 5 | 1.64 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 5 | 1.64 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 5 | 1.64 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 5 | 1.64 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 5 | 1.64 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 5 | 1.64 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 5 | 1.64 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 5 | 1.64 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE1 | 6 | 1.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE2 | 6 | 1.64 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE3 | 6 | 1.64 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 18 | 1.64 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 18 | 1.64 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 18 | 1.64 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 19 | 1.64 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 5 | 1.64 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 5 | 1.64 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 5 | 1.64 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 19 | 1.64 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 19 | 1.64 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 19 | 1.64 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 6 | 1.64 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 6 | 1.64 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 6 | 1.64 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 6 | 1.64 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 6 | 1.64 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 6 | 1.64 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 6 | 1.64 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 6 | 1.64 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 6 | 1.64 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 18 | 1.64 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 18 | 1.64 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 18 | 1.64 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 18 | 1.64 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 18 | 1.64 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 18 | 1.64 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 11 | 1.64 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 11 | 1.64 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 11 | 1.64 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 17 | 1.64 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 17 | 1.64 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 17 | 1.64 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 11 | 1.64 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 11 | 1.64 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 14 | 1.64 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 14 | 1.64 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 14 | 1.64 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 12 | 1.64 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 12 | 1.64 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 12 | 1.64 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 15 | 1.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 15 | 1.64 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 15 | 1.64 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 17 | 1.64 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 17 | 1.64 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 17 | 1.64 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 6 | 1.64 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 6 | 1.64 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 6 | 1.64 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 2 | 1.64 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 12 | 1.64 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 5 | 1.64 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 5 | 1.64 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 5 | 1.64 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 18 | 1.63 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 18 | 1.63 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 10 | 1.63 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 10 | 1.63 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 10 | 1.63 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 18 | 1.63 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 18 | 1.63 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 18 | 1.63 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 2 | 1.63 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 17 | 1.63 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 4 | 1.63 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 4 | 1.63 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 4 | 1.63 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 19 | 1.63 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 1 | 1.63 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 1 | 1.63 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 1 | 1.63 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 11 | 1.63 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 11 | 1.63 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 11 | 1.63 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 1 | 1.63 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 1 | 1.63 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 1 | 1.63 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 6 | 1.63 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 6 | 1.63 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 6 | 1.63 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 6 | 1.63 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 6 | 1.63 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 6 | 1.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 13 | 1.63 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 13 | 1.63 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 13 | 1.63 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 18 | 1.63 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 9 | 1.63 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 9 | 1.63 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 9 | 1.63 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 7 | 1.63 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 7 | 1.63 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 7 | 1.63 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 14 | 1.63 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 14 | 1.63 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 14 | 1.63 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 13 | 1.63 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 13 | 1.63 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 13 | 1.63 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 13 | 1.63 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 13 | 1.63 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 13 | 1.63 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 2 | 1.63 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 14 | 1.63 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 7 | 1.63 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 7 | 1.63 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 7 | 1.63 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 9 | 1.63 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 9 | 1.63 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 9 | 1.63 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 16 | 1.63 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 16 | 1.63 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 16 | 1.63 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 6 | 1.63 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 14 | 1.63 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 1 | 1.62 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 1 | 1.62 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 1 | 1.62 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 1 | 1.62 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 1 | 1.62 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 1 | 1.62 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG11 | 2 | 1.62 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG12 | 2 | 1.62 |
| (1,3380) | 1:34:A:TYR:HD1 | 1:39:A:VAL:HG13 | 2 | 1.62 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG11 | 2 | 1.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG12 | 2 | 1.62 |
| (1,3380) | 1:34:A:TYR:HD2 | 1:39:A:VAL:HG13 | 2 | 1.62 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 13 | 1.62 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 9 | 1.62 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 9 | 1.62 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 9 | 1.62 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 19 | 1.62 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 19 | 1.62 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 19 | 1.62 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 3 | 1.62 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 13 | 1.62 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 4 | 1.62 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 4 | 1.62 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 4 | 1.62 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 4 | 1.62 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 4 | 1.62 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 4 | 1.62 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 4 | 1.62 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 4 | 1.62 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 4 | 1.62 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 7 | 1.62 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 7 | 1.62 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 7 | 1.62 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 10 | 1.62 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 10 | 1.62 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 10 | 1.62 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 10 | 1.62 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 10 | 1.62 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 10 | 1.62 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 10 | 1.62 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 10 | 1.62 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 10 | 1.62 |
| (1,2441) | 1:119:A:GLU:HA | 1:122:A:ASP:HB3 | 6 | 1.62 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 12 | 1.62 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 12 | 1.62 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 12 | 1.62 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 5 | 1.62 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 14 | 1.62 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 14 | 1.62 |
| (1,1916) | 1:91:A:MET:HB2 | 1:92:A:PHE:HE1 | 13 | 1.62 |
| (1,1916) | 1:91:A:MET:HB2 | 1:92:A:PHE:HE2 | 13 | 1.62 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 10 | 1.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 10 | 1.62 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 10 | 1.62 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 19 | 1.62 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 19 | 1.62 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 19 | 1.62 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 15 | 1.62 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 15 | 1.62 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 15 | 1.62 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 19 | 1.62 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 19 | 1.62 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 19 | 1.62 |
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 4 | 1.61 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 4 | 1.61 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 11 | 1.61 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 11 | 1.61 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 11 | 1.61 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 1 | 1.61 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 8 | 1.61 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 6 | 1.61 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 6 | 1.61 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 6 | 1.61 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 10 | 1.61 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 10 | 1.61 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 10 | 1.61 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 5 | 1.61 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 20 | 1.61 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 20 | 1.61 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 20 | 1.61 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 7 | 1.61 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 7 | 1.61 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 7 | 1.61 |
| (1,1545) | 1:186:A:GLU:HG3 | 1:187:A:LYS:HD3 | 11 | 1.61 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 13 | 1.61 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 13 | 1.61 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 13 | 1.61 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 19 | 1.61 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 19 | 1.61 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 19 | 1.61 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 1 | 1.61 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 1 | 1.61 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 1 | 1.61 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 2 | 1.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 2 | 1.61 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 2 | 1.61 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 17 | 1.61 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 17 | 1.61 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 17 | 1.61 |
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 15 | 1.6 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 15 | 1.6 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 11 | 1.6 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 11 | 1.6 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 11 | 1.6 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 11 | 1.6 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 11 | 1.6 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 11 | 1.6 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 11 | 1.6 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 11 | 1.6 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 11 | 1.6 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 18 | 1.6 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 18 | 1.6 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 18 | 1.6 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 9 | 1.6 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 9 | 1.6 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 9 | 1.6 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 9 | 1.6 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 9 | 1.6 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 9 | 1.6 |
| (1,2441) | 1:119:A:GLU:HA | 1:122:A:ASP:HB3 | 13 | 1.6 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 20 | 1.6 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 20 | 1.6 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 20 | 1.6 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 20 | 1.6 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 20 | 1.6 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 20 | 1.6 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 20 | 1.6 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 20 | 1.6 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 20 | 1.6 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 16 | 1.6 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 7 | 1.6 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 7 | 1.6 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 7 | 1.6 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 7 | 1.6 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 7 | 1.6 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 7 | 1.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 10 | 1.6 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 10 | 1.6 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 10 | 1.6 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 19 | 1.6 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 19 | 1.6 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 19 | 1.6 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 10 | 1.6 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 10 | 1.6 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 10 | 1.6 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 9 | 1.6 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 9 | 1.6 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 9 | 1.6 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 3 | 1.6 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 3 | 1.6 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 3 | 1.6 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 10 | 1.6 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 10 | 1.6 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 10 | 1.6 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 12 | 1.6 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 12 | 1.6 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 12 | 1.6 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 1 | 1.6 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 1 | 1.6 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 1 | 1.6 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 14 | 1.6 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 14 | 1.6 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 14 | 1.6 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 5 | 1.6 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 5 | 1.6 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 5 | 1.6 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 10 | 1.6 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 10 | 1.6 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 10 | 1.6 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 9 | 1.59 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 9 | 1.59 |
| (1,3279) | 1:116:A:VAL:HG21 | 1:118:A:GLY:HA3 | 4 | 1.59 |
| (1,3279) | 1:116:A:VAL:HG22 | 1:118:A:GLY:HA3 | 4 | 1.59 |
| (1,3279) | 1:116:A:VAL:HG23 | 1:118:A:GLY:HA3 | 4 | 1.59 |
| (1,3107) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HB2 | 13 | 1.59 |
| (1,3107) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HB2 | 13 | 1.59 |
| (1,3107) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HB2 | 13 | 1.59 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 2 | 1.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 2 | 1.59 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 2 | 1.59 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 18 | 1.59 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 20 | 1.59 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 20 | 1.59 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 20 | 1.59 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 20 | 1.59 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 20 | 1.59 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 20 | 1.59 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 20 | 1.59 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 20 | 1.59 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 20 | 1.59 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 8 | 1.59 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 8 | 1.59 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 8 | 1.59 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 14 | 1.59 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 14 | 1.59 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 14 | 1.59 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 6 | 1.59 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 6 | 1.59 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 6 | 1.59 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 3 | 1.59 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 3 | 1.59 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 3 | 1.59 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 3 | 1.59 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 3 | 1.59 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 3 | 1.59 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 3 | 1.59 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 3 | 1.59 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 3 | 1.59 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 7 | 1.59 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 7 | 1.59 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 7 | 1.59 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 12 | 1.59 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 12 | 1.59 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 12 | 1.59 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 7 | 1.59 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 12 | 1.59 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 12 | 1.59 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 12 | 1.59 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 18 | 1.59 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 18 | 1.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 18 | 1.59 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 6 | 1.59 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 6 | 1.59 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 6 | 1.59 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 10 | 1.59 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 10 | 1.59 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 10 | 1.59 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 11 | 1.59 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 11 | 1.59 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 11 | 1.59 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 7 | 1.59 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 7 | 1.59 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 7 | 1.59 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 6 | 1.59 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 6 | 1.59 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 6 | 1.59 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 17 | 1.58 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 17 | 1.58 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 17 | 1.58 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 2 | 1.58 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 2 | 1.58 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 2 | 1.58 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 16 | 1.58 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 16 | 1.58 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 16 | 1.58 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 14 | 1.58 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 14 | 1.58 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 14 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 12 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 12 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 12 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 12 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 12 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 12 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 17 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 17 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 17 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 17 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 17 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 17 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 20 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 20 | 1.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 20 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 20 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 20 | 1.58 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 20 | 1.58 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 20 | 1.58 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 20 | 1.58 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 4 | 1.58 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 4 | 1.58 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 4 | 1.58 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 20 | 1.58 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 20 | 1.58 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 20 | 1.58 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 20 | 1.58 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 20 | 1.58 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 20 | 1.58 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 19 | 1.58 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 19 | 1.58 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 19 | 1.58 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 10 | 1.58 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 10 | 1.58 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 10 | 1.58 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 13 | 1.58 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 13 | 1.58 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 13 | 1.58 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 5 | 1.58 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 5 | 1.58 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 5 | 1.58 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 17 | 1.58 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 17 | 1.58 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 17 | 1.58 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 20 | 1.58 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 20 | 1.58 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 20 | 1.58 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 8 | 1.58 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 8 | 1.58 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 8 | 1.58 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 12 | 1.58 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 12 | 1.58 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 12 | 1.58 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 16 | 1.58 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 16 | 1.58 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 16 | 1.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 18 | 1.58 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 18 | 1.58 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 18 | 1.58 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 14 | 1.58 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 14 | 1.58 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 14 | 1.58 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 8 | 1.57 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 8 | 1.57 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 8 | 1.57 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 8 | 1.57 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 8 | 1.57 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 8 | 1.57 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 20 | 1.57 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 20 | 1.57 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 20 | 1.57 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 3 | 1.57 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 3 | 1.57 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 3 | 1.57 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 18 | 1.57 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 18 | 1.57 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 18 | 1.57 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 6 | 1.57 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 1 | 1.57 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 1 | 1.57 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 1 | 1.57 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 1 | 1.57 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 1 | 1.57 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 1 | 1.57 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 6 | 1.57 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 6 | 1.57 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 6 | 1.57 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 6 | 1.57 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 6 | 1.57 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 6 | 1.57 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 4 | 1.57 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 4 | 1.57 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 4 | 1.57 |
| (1,1715) | 1:133:A:LEU:H | 1:136:A:GLN:HG2 | 12 | 1.57 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 6 | 1.57 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 6 | 1.57 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 6 | 1.57 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 2 | 1.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 2 | 1.57 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 2 | 1.57 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 3 | 1.57 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 3 | 1.57 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 3 | 1.57 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 5 | 1.57 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 5 | 1.57 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 5 | 1.57 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 8 | 1.57 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 8 | 1.57 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 8 | 1.57 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 16 | 1.57 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 16 | 1.57 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 16 | 1.57 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 17 | 1.57 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 7 | 1.57 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 7 | 1.57 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 7 | 1.57 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 3 | 1.57 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 3 | 1.57 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 3 | 1.57 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 7 | 1.57 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 7 | 1.57 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 7 | 1.57 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 8 | 1.57 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 8 | 1.57 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 8 | 1.57 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 19 | 1.57 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 1 | 1.57 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 1 | 1.57 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 1 | 1.57 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 6 | 1.57 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 6 | 1.57 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 6 | 1.57 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 4 | 1.56 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 4 | 1.56 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 4 | 1.56 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 17 | 1.56 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 17 | 1.56 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 17 | 1.56 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 17 | 1.56 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 17 | 1.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 17 | 1.56 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 17 | 1.56 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 17 | 1.56 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 17 | 1.56 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 7 | 1.56 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 11 | 1.56 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 12 | 1.56 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 3 | 1.56 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 3 | 1.56 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 3 | 1.56 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 19 | 1.56 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 19 | 1.56 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 19 | 1.56 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 16 | 1.56 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 16 | 1.56 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 16 | 1.56 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 7 | 1.56 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 7 | 1.56 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 7 | 1.56 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 3 | 1.56 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 3 | 1.56 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 3 | 1.56 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 3 | 1.56 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 3 | 1.56 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 3 | 1.56 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 3 | 1.56 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 3 | 1.56 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 3 | 1.56 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 3 | 1.56 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 3 | 1.56 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 3 | 1.56 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 5 | 1.56 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 5 | 1.56 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 5 | 1.56 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 2 | 1.56 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 2 | 1.56 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 2 | 1.56 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 2 | 1.56 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 2 | 1.56 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 2 | 1.56 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 2 | 1.56 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 2 | 1.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 2 | 1.56 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 1 | 1.56 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 1 | 1.56 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 1 | 1.56 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 1 | 1.56 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 1 | 1.56 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 1 | 1.56 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 1 | 1.56 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 1 | 1.56 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 1 | 1.56 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 1 | 1.56 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 1 | 1.56 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 1 | 1.56 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 4 | 1.56 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 4 | 1.56 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 16 | 1.56 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 19 | 1.56 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 19 | 1.56 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 10 | 1.56 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 10 | 1.56 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 10 | 1.56 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 10 | 1.56 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 10 | 1.56 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 10 | 1.56 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 12 | 1.56 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 12 | 1.56 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 12 | 1.56 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 4 | 1.56 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 4 | 1.56 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 4 | 1.56 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 20 | 1.56 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 20 | 1.56 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 20 | 1.56 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG11 | 8 | 1.56 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG12 | 8 | 1.56 |
| (1,603) | 1:184:A:LEU:H | 1:185:A:VAL:HG13 | 8 | 1.56 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 19 | 1.56 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 19 | 1.56 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 19 | 1.56 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 20 | 1.56 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 20 | 1.56 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 20 | 1.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 9 | 1.56 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 9 | 1.56 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 9 | 1.56 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 1 | 1.56 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 1 | 1.56 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 1 | 1.56 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 19 | 1.55 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 19 | 1.55 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 19 | 1.55 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 19 | 1.55 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 19 | 1.55 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 19 | 1.55 |
| (1,3107) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HB2 | 15 | 1.55 |
| (1,3107) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HB2 | 15 | 1.55 |
| (1,3107) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HB2 | 15 | 1.55 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 12 | 1.55 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 12 | 1.55 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 12 | 1.55 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 9 | 1.55 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 9 | 1.55 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 9 | 1.55 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 8 | 1.55 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 8 | 1.55 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 8 | 1.55 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 8 | 1.55 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 8 | 1.55 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 8 | 1.55 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 8 | 1.55 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 8 | 1.55 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 8 | 1.55 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 6 | 1.55 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 6 | 1.55 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 6 | 1.55 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 1 | 1.55 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 1 | 1.55 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 1 | 1.55 |
| (1,1351) | 1:179:A:ASP:HB2 | 1:183:A:GLN:HE21 | 8 | 1.55 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 6 | 1.55 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 8 | 1.55 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 8 | 1.55 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 8 | 1.55 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 8 | 1.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 8 | 1.55 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 8 | 1.55 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 9 | 1.55 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 9 | 1.55 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 9 | 1.55 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 20 | 1.55 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 18 | 1.55 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 18 | 1.55 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 18 | 1.55 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 10 | 1.55 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 10 | 1.55 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 10 | 1.55 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 19 | 1.55 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 19 | 1.55 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 19 | 1.55 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG11 | 7 | 1.54 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG12 | 7 | 1.54 |
| (1,3004) | 1:94:A:ALA:HA | 1:95:A:VAL:HG13 | 7 | 1.54 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 20 | 1.54 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 16 | 1.54 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 16 | 1.54 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 16 | 1.54 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 2 | 1.54 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 2 | 1.54 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 2 | 1.54 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 14 | 1.54 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 14 | 1.54 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 14 | 1.54 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 10 | 1.54 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 2 | 1.54 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 9 | 1.54 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 4 | 1.54 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 4 | 1.54 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 4 | 1.54 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 4 | 1.54 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 4 | 1.54 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 4 | 1.54 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 14 | 1.54 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 13 | 1.54 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 13 | 1.54 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 13 | 1.54 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 13 | 1.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 13 | 1.54 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 13 | 1.54 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 13 | 1.54 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 13 | 1.54 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 13 | 1.54 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 15 | 1.54 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 15 | 1.54 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 15 | 1.54 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 15 | 1.54 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 15 | 1.54 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 15 | 1.54 |
| (1,778) | 1:51:A:PRO:HB3 | 1:54:A:THR:H | 5 | 1.54 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 4 | 1.54 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 4 | 1.54 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 4 | 1.54 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 16 | 1.54 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 19 | 1.54 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 19 | 1.54 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 19 | 1.54 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 20 | 1.54 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 20 | 1.54 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 20 | 1.54 |
| (1,3527) | 1:73:A:GLN:HG2 | 1:125:A:TRP:HZ2 | 16 | 1.53 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 17 | 1.53 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 17 | 1.53 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 5 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 13 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 13 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 13 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 13 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 13 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 13 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 13 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 13 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 13 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 14 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 14 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 14 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 14 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 14 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 14 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 14 | 1.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 14 | 1.53 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 14 | 1.53 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 5 | 1.53 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 5 | 1.53 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 5 | 1.53 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 5 | 1.53 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 5 | 1.53 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 5 | 1.53 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 5 | 1.53 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 5 | 1.53 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 5 | 1.53 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 10 | 1.53 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 10 | 1.53 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 10 | 1.53 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 12 | 1.53 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 12 | 1.53 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 12 | 1.53 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 18 | 1.53 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 18 | 1.53 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 18 | 1.53 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 20 | 1.53 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 6 | 1.53 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 6 | 1.53 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 6 | 1.53 |
| (1,2017) | 1:117:A:LYS:HD3 | 1:120:A:ASP:H | 12 | 1.53 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 8 | 1.53 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 16 | 1.53 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 16 | 1.53 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 4 | 1.53 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 4 | 1.53 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 4 | 1.53 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 1 | 1.53 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 1 | 1.53 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 1 | 1.53 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 4 | 1.53 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 4 | 1.53 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 4 | 1.53 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 4 | 1.53 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 4 | 1.53 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 4 | 1.53 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 18 | 1.53 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 18 | 1.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 18 | 1.53 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 1 | 1.53 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 1 | 1.53 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 1 | 1.53 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 4 | 1.53 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 4 | 1.53 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 4 | 1.53 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 4 | 1.53 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 1 | 1.53 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 1 | 1.53 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 1 | 1.53 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 15 | 1.53 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 15 | 1.53 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 15 | 1.53 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 17 | 1.52 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 17 | 1.52 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 17 | 1.52 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 17 | 1.52 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 17 | 1.52 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 17 | 1.52 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 1 | 1.52 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 1 | 1.52 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 1 | 1.52 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 1 | 1.52 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 1 | 1.52 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 1 | 1.52 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 1 | 1.52 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 1 | 1.52 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 1 | 1.52 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 12 | 1.52 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 12 | 1.52 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 12 | 1.52 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 12 | 1.52 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 15 | 1.52 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 15 | 1.52 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 15 | 1.52 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 3 | 1.52 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 3 | 1.52 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 3 | 1.52 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 15 | 1.52 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 15 | 1.52 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 15 | 1.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 9 | 1.52 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 9 | 1.52 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 9 | 1.52 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 2 | 1.52 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 2 | 1.52 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 2 | 1.52 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 13 | 1.52 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 13 | 1.52 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 13 | 1.52 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 8 | 1.52 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 8 | 1.52 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 8 | 1.52 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 16 | 1.52 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 16 | 1.52 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 16 | 1.52 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 1 | 1.52 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 1 | 1.52 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 1 | 1.52 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 12 | 1.52 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 8 | 1.52 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 8 | 1.52 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 8 | 1.52 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 8 | 1.52 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 8 | 1.52 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 8 | 1.52 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 17 | 1.52 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 7 | 1.52 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 7 | 1.52 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 7 | 1.52 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 18 | 1.52 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 18 | 1.52 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 18 | 1.52 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 18 | 1.52 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 18 | 1.52 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 18 | 1.52 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 19 | 1.52 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 19 | 1.52 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 19 | 1.52 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 16 | 1.52 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 16 | 1.52 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 16 | 1.52 |
| (1,102) | 1:50:A:LEU:HD21 | 1:56:A:MET:H | 17 | 1.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,102) | 1:50:A:LEU:HD22 | 1:56:A:MET:H | 17 | 1.52 |
| (1,102) | 1:50:A:LEU:HD23 | 1:56:A:MET:H | 17 | 1.52 |
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 7 | 1.51 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 7 | 1.51 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 14 | 1.51 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 1 | 1.51 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 1 | 1.51 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 1 | 1.51 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 8 | 1.51 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 8 | 1.51 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 8 | 1.51 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 8 | 1.51 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 8 | 1.51 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 8 | 1.51 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 8 | 1.51 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 8 | 1.51 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 8 | 1.51 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 9 | 1.51 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 9 | 1.51 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 9 | 1.51 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 17 | 1.51 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 17 | 1.51 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 17 | 1.51 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 8 | 1.51 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 8 | 1.51 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 8 | 1.51 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 18 | 1.51 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 18 | 1.51 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 18 | 1.51 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 19 | 1.51 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 19 | 1.51 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 19 | 1.51 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 17 | 1.51 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 17 | 1.51 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 17 | 1.51 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 17 | 1.51 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 17 | 1.51 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 17 | 1.51 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 17 | 1.51 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 17 | 1.51 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 17 | 1.51 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 6 | 1.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 6 | 1.51 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 6 | 1.51 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 6 | 1.51 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 18 | 1.51 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 18 | 1.51 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 18 | 1.51 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 14 | 1.51 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 7 | 1.51 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 7 | 1.51 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 7 | 1.51 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 7 | 1.51 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 7 | 1.51 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 7 | 1.51 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 11 | 1.51 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 11 | 1.51 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 11 | 1.51 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 20 | 1.51 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 3 | 1.5 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 11 | 1.5 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 14 | 1.5 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 14 | 1.5 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 14 | 1.5 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 14 | 1.5 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 14 | 1.5 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 14 | 1.5 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 1 | 1.5 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 1 | 1.5 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 1 | 1.5 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 4 | 1.5 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 4 | 1.5 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 4 | 1.5 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 4 | 1.5 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 4 | 1.5 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 4 | 1.5 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 4 | 1.5 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 4 | 1.5 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 4 | 1.5 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 15 | 1.5 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 15 | 1.5 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 15 | 1.5 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 18 | 1.5 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 18 | 1.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 18 | 1.5 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 3 | 1.5 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 3 | 1.5 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 3 | 1.5 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 18 | 1.5 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 18 | 1.5 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 18 | 1.5 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 13 | 1.5 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 13 | 1.5 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 13 | 1.5 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 13 | 1.5 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 13 | 1.5 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 13 | 1.5 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 13 | 1.5 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 13 | 1.5 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 13 | 1.5 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 13 | 1.5 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 13 | 1.5 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 13 | 1.5 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 11 | 1.5 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 11 | 1.5 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 11 | 1.5 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 10 | 1.5 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 10 | 1.5 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 10 | 1.5 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 10 | 1.5 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 10 | 1.5 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 10 | 1.5 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 10 | 1.5 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 10 | 1.5 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 10 | 1.5 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 3 | 1.5 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 3 | 1.5 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 3 | 1.5 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 4 | 1.5 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 4 | 1.5 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 4 | 1.5 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 17 | 1.5 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 17 | 1.5 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 17 | 1.5 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 17 | 1.5 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 17 | 1.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 17 | 1.5 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 8 | 1.5 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 9 | 1.5 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 18 | 1.5 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 11 | 1.5 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 11 | 1.5 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 11 | 1.5 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 14 | 1.5 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 14 | 1.5 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 14 | 1.5 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 13 | 1.5 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 13 | 1.5 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 13 | 1.5 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 17 | 1.49 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 17 | 1.49 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 17 | 1.49 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 12 | 1.49 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 12 | 1.49 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 12 | 1.49 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 12 | 1.49 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 12 | 1.49 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 12 | 1.49 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 12 | 1.49 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 12 | 1.49 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 12 | 1.49 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 14 | 1.49 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 14 | 1.49 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 14 | 1.49 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 18 | 1.49 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 18 | 1.49 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 18 | 1.49 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 12 | 1.49 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 12 | 1.49 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 12 | 1.49 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 12 | 1.49 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 12 | 1.49 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 12 | 1.49 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 12 | 1.49 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 12 | 1.49 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 12 | 1.49 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 11 | 1.49 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 11 | 1.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 11 | 1.49 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 9 | 1.49 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 9 | 1.49 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 9 | 1.49 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 8 | 1.49 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 8 | 1.49 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 8 | 1.49 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 8 | 1.49 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 8 | 1.49 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 8 | 1.49 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 8 | 1.49 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 8 | 1.49 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 8 | 1.49 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 15 | 1.49 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 15 | 1.49 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 15 | 1.49 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 19 | 1.49 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 19 | 1.49 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 19 | 1.49 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 17 | 1.49 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 9 | 1.49 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 9 | 1.49 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 9 | 1.49 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 9 | 1.49 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 9 | 1.49 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 9 | 1.49 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 14 | 1.49 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 14 | 1.49 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 14 | 1.49 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 14 | 1.49 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 14 | 1.49 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 14 | 1.49 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 9 | 1.49 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 9 | 1.49 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 9 | 1.49 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG21 | 18 | 1.49 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG22 | 18 | 1.49 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG23 | 18 | 1.49 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG21 | 18 | 1.49 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG22 | 18 | 1.49 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG23 | 18 | 1.49 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 4 | 1.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 4 | 1.49 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 4 | 1.49 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 14 | 1.49 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 14 | 1.49 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 14 | 1.49 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 5 | 1.49 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 5 | 1.49 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 5 | 1.49 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 20 | 1.49 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 20 | 1.49 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 20 | 1.49 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 17 | 1.49 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 18 | 1.49 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 3 | 1.49 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 3 | 1.49 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 3 | 1.49 |
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 17 | 1.48 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 1 | 1.48 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 1 | 1.48 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 1 | 1.48 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 8 | 1.48 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 20 | 1.48 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 20 | 1.48 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 20 | 1.48 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 10 | 1.48 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 10 | 1.48 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 10 | 1.48 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 11 | 1.48 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 11 | 1.48 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 11 | 1.48 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 18 | 1.48 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 18 | 1.48 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 18 | 1.48 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 14 | 1.48 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 20 | 1.48 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 2 | 1.48 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 2 | 1.48 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 2 | 1.48 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 2 | 1.48 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 2 | 1.48 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 2 | 1.48 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 10 | 1.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 10 | 1.48 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 10 | 1.48 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 10 | 1.48 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 10 | 1.48 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 10 | 1.48 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 2 | 1.48 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 13 | 1.48 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 13 | 1.48 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 13 | 1.48 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 11 | 1.48 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 11 | 1.48 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 11 | 1.48 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 18 | 1.48 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 18 | 1.48 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 7 | 1.48 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 7 | 1.48 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 7 | 1.48 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 7 | 1.48 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 7 | 1.48 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 3 | 1.48 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 7 | 1.48 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 20 | 1.48 |
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 7 | 1.47 |
| (1,3480) | 1:32:A:HIS:HD2 | 1:150:A:PRO:HG3 | 10 | 1.47 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 5 | 1.47 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 5 | 1.47 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 5 | 1.47 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 5 | 1.47 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 5 | 1.47 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 5 | 1.47 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 5 | 1.47 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 5 | 1.47 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 5 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 9 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 9 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 9 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 9 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 9 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 9 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 9 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 9 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 9 | 1.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 13 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 13 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 13 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 13 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 13 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 13 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 13 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 13 | 1.47 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 13 | 1.47 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 10 | 1.47 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 10 | 1.47 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 10 | 1.47 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 10 | 1.47 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 10 | 1.47 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 10 | 1.47 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 10 | 1.47 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 10 | 1.47 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 10 | 1.47 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 13 | 1.47 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 13 | 1.47 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 13 | 1.47 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 17 | 1.47 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 17 | 1.47 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 17 | 1.47 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 9 | 1.47 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 9 | 1.47 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 9 | 1.47 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 16 | 1.47 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 16 | 1.47 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 16 | 1.47 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 11 | 1.47 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 11 | 1.47 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 11 | 1.47 |
| (1,2441) | 1:119:A:GLU:HA | 1:122:A:ASP:HB3 | 7 | 1.47 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 10 | 1.47 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 10 | 1.47 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 10 | 1.47 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 15 | 1.47 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 15 | 1.47 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 15 | 1.47 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 15 | 1.47 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 15 | 1.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 15 | 1.47 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 18 | 1.47 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 18 | 1.47 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 18 | 1.47 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 16 | 1.47 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 16 | 1.47 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 16 | 1.47 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 18 | 1.47 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 18 | 1.47 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 18 | 1.47 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG21 | 19 | 1.47 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG22 | 19 | 1.47 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG23 | 19 | 1.47 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG21 | 19 | 1.47 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG22 | 19 | 1.47 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG23 | 19 | 1.47 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 3 | 1.47 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 1 | 1.47 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 1 | 1.47 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 1 | 1.47 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 1 | 1.47 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 1 | 1.47 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 1 | 1.47 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 18 | 1.47 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 18 | 1.47 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 18 | 1.47 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 9 | 1.46 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 9 | 1.46 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 9 | 1.46 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 9 | 1.46 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 9 | 1.46 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 9 | 1.46 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 9 | 1.46 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 9 | 1.46 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 9 | 1.46 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 18 | 1.46 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 6 | 1.46 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 6 | 1.46 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 6 | 1.46 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 6 | 1.46 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 6 | 1.46 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 6 | 1.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 6 | 1.46 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 6 | 1.46 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 6 | 1.46 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 2 | 1.46 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 2 | 1.46 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 2 | 1.46 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 4 | 1.46 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 4 | 1.46 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 4 | 1.46 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 12 | 1.46 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 12 | 1.46 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 12 | 1.46 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 11 | 1.46 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 11 | 1.46 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 11 | 1.46 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 7 | 1.46 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 7 | 1.46 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 7 | 1.46 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 5 | 1.46 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 17 | 1.46 |
| (1,1578) | 1:118:A:GLY:H | 1:119:A:GLU:HG3 | 3 | 1.46 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 18 | 1.46 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 18 | 1.46 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 18 | 1.46 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 8 | 1.46 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 8 | 1.46 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 8 | 1.46 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 6 | 1.46 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 6 | 1.46 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 6 | 1.46 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 5 | 1.46 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 5 | 1.46 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 5 | 1.46 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 5 | 1.46 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 5 | 1.46 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 5 | 1.46 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 15 | 1.46 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 10 | 1.46 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 10 | 1.46 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 10 | 1.46 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 18 | 1.46 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 15 | 1.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 15 | 1.46 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 15 | 1.46 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 14 | 1.46 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 6 | 1.46 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 6 | 1.46 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 6 | 1.46 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 1 | 1.46 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 1 | 1.46 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 1 | 1.46 |
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 19 | 1.45 |
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 10 | 1.45 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 10 | 1.45 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 14 | 1.45 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 14 | 1.45 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 14 | 1.45 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 14 | 1.45 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 14 | 1.45 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 14 | 1.45 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 14 | 1.45 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 14 | 1.45 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 14 | 1.45 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG11 | 12 | 1.45 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG12 | 12 | 1.45 |
| (1,2579) | 1:91:A:MET:HA | 1:95:A:VAL:HG13 | 12 | 1.45 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 10 | 1.45 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 10 | 1.45 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 10 | 1.45 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 15 | 1.45 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 19 | 1.45 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 6 | 1.45 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 6 | 1.45 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 6 | 1.45 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 6 | 1.45 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 6 | 1.45 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 6 | 1.45 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 6 | 1.45 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 6 | 1.45 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 6 | 1.45 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG11 | 18 | 1.45 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG12 | 18 | 1.45 |
| (1,2169) | 1:40:A:LEU:HG | 1:42:A:VAL:HG13 | 18 | 1.45 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 5 | 1.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 5 | 1.45 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 5 | 1.45 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 5 | 1.45 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 5 | 1.45 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 5 | 1.45 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 10 | 1.45 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 10 | 1.45 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 3 | 1.45 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 10 | 1.45 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 10 | 1.45 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 10 | 1.45 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 16 | 1.45 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 16 | 1.45 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 16 | 1.45 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 9 | 1.45 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 9 | 1.45 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 9 | 1.45 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 9 | 1.45 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 9 | 1.45 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 9 | 1.45 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 4 | 1.45 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 7 | 1.45 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 5 | 1.45 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 5 | 1.45 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 5 | 1.45 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 9 | 1.45 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 9 | 1.45 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 9 | 1.45 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 4 | 1.45 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 9 | 1.45 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 5 | 1.45 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 14 | 1.45 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 14 | 1.45 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 14 | 1.45 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 17 | 1.45 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 17 | 1.45 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 17 | 1.45 |
| (1,199) | 1:116:A:VAL:HG21 | 1:121:A:TYR:H | 5 | 1.45 |
| (1,199) | 1:116:A:VAL:HG22 | 1:121:A:TYR:H | 5 | 1.45 |
| (1,199) | 1:116:A:VAL:HG23 | 1:121:A:TYR:H | 5 | 1.45 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 7 | 1.44 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 7 | 1.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 7 | 1.44 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 7 | 1.44 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 7 | 1.44 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 7 | 1.44 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 6 | 1.44 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 6 | 1.44 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 6 | 1.44 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 6 | 1.44 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 6 | 1.44 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 6 | 1.44 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 14 | 1.44 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 14 | 1.44 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 14 | 1.44 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 10 | 1.44 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 10 | 1.44 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 10 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 2 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 2 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 2 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 2 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 2 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 2 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 2 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 2 | 1.44 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 2 | 1.44 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 7 | 1.44 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 7 | 1.44 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 7 | 1.44 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 14 | 1.44 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 14 | 1.44 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 14 | 1.44 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 16 | 1.44 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 16 | 1.44 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 16 | 1.44 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 12 | 1.44 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 13 | 1.44 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 17 | 1.44 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 17 | 1.44 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 17 | 1.44 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 17 | 1.44 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 3 | 1.44 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 17 | 1.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 11 | 1.44 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 11 | 1.44 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 11 | 1.44 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 2 | 1.44 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 2 | 1.44 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 2 | 1.44 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 9 | 1.44 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 9 | 1.44 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 9 | 1.44 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 16 | 1.44 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 16 | 1.44 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 16 | 1.44 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 9 | 1.44 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 9 | 1.44 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 9 | 1.44 |
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 1 | 1.43 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 13 | 1.43 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 13 | 1.43 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 13 | 1.43 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 13 | 1.43 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 13 | 1.43 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 13 | 1.43 |
| (1,3480) | 1:32:A:HIS:HD2 | 1:150:A:PRO:HG3 | 4 | 1.43 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 18 | 1.43 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 1 | 1.43 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 1 | 1.43 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 1 | 1.43 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 4 | 1.43 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 4 | 1.43 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 4 | 1.43 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 17 | 1.43 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 17 | 1.43 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 17 | 1.43 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 7 | 1.43 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 7 | 1.43 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 7 | 1.43 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 7 | 1.43 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 7 | 1.43 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 7 | 1.43 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 7 | 1.43 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 7 | 1.43 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 7 | 1.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 7 | 1.43 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 7 | 1.43 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 7 | 1.43 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 15 | 1.43 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 15 | 1.43 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 15 | 1.43 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 16 | 1.43 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 16 | 1.43 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 16 | 1.43 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 13 | 1.43 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 13 | 1.43 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 13 | 1.43 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 4 | 1.43 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 9 | 1.43 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 9 | 1.43 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 9 | 1.43 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 9 | 1.43 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 9 | 1.43 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 9 | 1.43 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 4 | 1.43 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 4 | 1.43 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 4 | 1.43 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 9 | 1.43 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 9 | 1.43 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 9 | 1.43 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 9 | 1.43 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 9 | 1.43 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 9 | 1.43 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 11 | 1.43 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 11 | 1.43 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 11 | 1.43 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 16 | 1.43 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 3 | 1.43 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 3 | 1.43 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 3 | 1.43 |
| (1,1715) | 1:133:A:LEU:H | 1:136:A:GLN:HG2 | 8 | 1.43 |
| (1,1578) | 1:118:A:GLY:H | 1:119:A:GLU:HG3 | 12 | 1.43 |
| (1,1578) | 1:118:A:GLY:H | 1:119:A:GLU:HG3 | 20 | 1.43 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 15 | 1.43 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 15 | 1.43 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 15 | 1.43 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 3 | 1.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 3 | 1.43 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 3 | 1.43 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 9 | 1.43 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 6 | 1.43 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 6 | 1.43 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 6 | 1.43 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 3 | 1.43 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 3 | 1.43 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 3 | 1.43 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 17 | 1.43 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 17 | 1.43 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 17 | 1.43 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 17 | 1.43 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 17 | 1.43 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 17 | 1.43 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 16 | 1.43 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 16 | 1.43 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 16 | 1.43 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 12 | 1.43 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 12 | 1.43 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 12 | 1.43 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 15 | 1.43 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 15 | 1.43 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 15 | 1.43 |
| (1,102) | 1:50:A:LEU:HD21 | 1:56:A:MET:H | 18 | 1.43 |
| (1,102) | 1:50:A:LEU:HD22 | 1:56:A:MET:H | 18 | 1.43 |
| (1,102) | 1:50:A:LEU:HD23 | 1:56:A:MET:H | 18 | 1.43 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 12 | 1.42 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 12 | 1.42 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 12 | 1.42 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG11 | 16 | 1.42 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG12 | 16 | 1.42 |
| (1,2881) | 1:40:A:LEU:HA | 1:42:A:VAL:HG13 | 16 | 1.42 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 8 | 1.42 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 8 | 1.42 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 8 | 1.42 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 8 | 1.42 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 8 | 1.42 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 8 | 1.42 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 8 | 1.42 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 8 | 1.42 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 8 | 1.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 10 | 1.42 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 10 | 1.42 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 10 | 1.42 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 18 | 1.42 |
| (1,2441) | 1:119:A:GLU:HA | 1:122:A:ASP:HB3 | 14 | 1.42 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 11 | 1.42 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 7 | 1.42 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 1 | 1.42 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 1 | 1.42 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 1 | 1.42 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 16 | 1.42 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 16 | 1.42 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 16 | 1.42 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 16 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 2 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 2 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 2 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 2 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 2 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 2 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 15 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 15 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 15 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 15 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 15 | 1.42 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 15 | 1.42 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 6 | 1.42 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 6 | 1.42 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 6 | 1.42 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 6 | 1.42 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 6 | 1.42 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 6 | 1.42 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 9 | 1.42 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 9 | 1.42 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 9 | 1.42 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 16 | 1.42 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 16 | 1.42 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 16 | 1.42 |
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 17 | 1.41 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 17 | 1.41 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 6 | 1.41 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 6 | 1.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 6 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 2 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 2 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 2 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 2 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 2 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 2 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 2 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 2 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 2 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 3 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 3 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 3 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 3 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 3 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 3 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 3 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 3 | 1.41 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 3 | 1.41 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 13 | 1.41 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 16 | 1.41 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 16 | 1.41 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 16 | 1.41 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 18 | 1.41 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 18 | 1.41 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 18 | 1.41 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 5 | 1.41 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 5 | 1.41 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 5 | 1.41 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 9 | 1.41 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 9 | 1.41 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 9 | 1.41 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 10 | 1.41 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 10 | 1.41 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 10 | 1.41 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 11 | 1.41 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 11 | 1.41 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 11 | 1.41 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 11 | 1.41 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 11 | 1.41 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 11 | 1.41 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 11 | 1.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 11 | 1.41 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 11 | 1.41 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 11 | 1.41 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 11 | 1.41 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 11 | 1.41 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 9 | 1.41 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 9 | 1.41 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 9 | 1.41 |
| (1,2017) | 1:117:A:LYS:HD3 | 1:120:A:ASP:H | 18 | 1.41 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 20 | 1.41 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 3 | 1.41 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 3 | 1.41 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 3 | 1.41 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 15 | 1.41 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 15 | 1.41 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 15 | 1.41 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 8 | 1.41 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 8 | 1.41 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 8 | 1.41 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 6 | 1.41 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 6 | 1.41 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 6 | 1.41 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 11 | 1.41 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 11 | 1.41 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 11 | 1.41 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 4 | 1.41 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 4 | 1.41 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 4 | 1.41 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 16 | 1.41 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 16 | 1.41 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 16 | 1.41 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 12 | 1.41 |
| (1,475) | 1:3:A:ILE:H | 1:8:A:GLN:HB2 | 15 | 1.41 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 4 | 1.4 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 4 | 1.4 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 4 | 1.4 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 4 | 1.4 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 4 | 1.4 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 4 | 1.4 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 17 | 1.4 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 17 | 1.4 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 8 | 1.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 8 | 1.4 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 8 | 1.4 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 16 | 1.4 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 16 | 1.4 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 16 | 1.4 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 8 | 1.4 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 8 | 1.4 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 8 | 1.4 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 8 | 1.4 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 8 | 1.4 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 8 | 1.4 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 10 | 1.4 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 10 | 1.4 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 10 | 1.4 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 18 | 1.4 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 18 | 1.4 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 18 | 1.4 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 15 | 1.4 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 15 | 1.4 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 15 | 1.4 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 15 | 1.4 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 15 | 1.4 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 15 | 1.4 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 15 | 1.4 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 15 | 1.4 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 15 | 1.4 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 9 | 1.4 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 16 | 1.4 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 16 | 1.4 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 16 | 1.4 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 5 | 1.4 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 5 | 1.4 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 5 | 1.4 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 3 | 1.4 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 3 | 1.4 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 3 | 1.4 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 16 | 1.4 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 16 | 1.4 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 16 | 1.4 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 4 | 1.4 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 4 | 1.4 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 4 | 1.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 14 | 1.4 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 8 | 1.4 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 8 | 1.4 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 8 | 1.4 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 13 | 1.4 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 20 | 1.4 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 20 | 1.4 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 20 | 1.4 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 20 | 1.4 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 20 | 1.4 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 20 | 1.4 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 20 | 1.4 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 2 | 1.4 |
| (1,1578) | 1:118:A:GLY:H | 1:119:A:GLU:HG3 | 4 | 1.4 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 7 | 1.4 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 7 | 1.4 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 7 | 1.4 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 16 | 1.4 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 16 | 1.4 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 16 | 1.4 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 16 | 1.4 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 16 | 1.4 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 16 | 1.4 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 20 | 1.4 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 20 | 1.4 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 20 | 1.4 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 12 | 1.4 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 12 | 1.4 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 12 | 1.4 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 10 | 1.4 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 15 | 1.39 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 15 | 1.39 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 15 | 1.39 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 9 | 1.39 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 2 | 1.39 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 2 | 1.39 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 2 | 1.39 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 9 | 1.39 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 9 | 1.39 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 9 | 1.39 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 14 | 1.39 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 14 | 1.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 14 | 1.39 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 18 | 1.39 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 18 | 1.39 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 18 | 1.39 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 13 | 1.39 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 15 | 1.39 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 15 | 1.39 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 15 | 1.39 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 14 | 1.39 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 14 | 1.39 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 14 | 1.39 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 4 | 1.39 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 19 | 1.39 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 12 | 1.39 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 15 | 1.39 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 15 | 1.39 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 15 | 1.39 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 19 | 1.39 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 17 | 1.39 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 17 | 1.39 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 17 | 1.39 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 12 | 1.39 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 12 | 1.39 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 12 | 1.39 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 13 | 1.39 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 13 | 1.39 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 13 | 1.39 |
| (1,1351) | 1:179:A:ASP:HB2 | 1:183:A:GLN:HE21 | 7 | 1.39 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 8 | 1.39 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 8 | 1.39 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 8 | 1.39 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 17 | 1.39 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 17 | 1.39 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 17 | 1.39 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 1 | 1.39 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 1 | 1.39 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 1 | 1.39 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 12 | 1.39 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 12 | 1.39 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 12 | 1.39 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 14 | 1.39 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 14 | 1.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 14 | 1.39 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG11 | 8 | 1.39 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG12 | 8 | 1.39 |
| (1,452) | 1:171:A:ASP:H | 1:172:A:VAL:HG13 | 8 | 1.39 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 14 | 1.39 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 14 | 1.39 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 14 | 1.39 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 19 | 1.38 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 19 | 1.38 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 19 | 1.38 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 19 | 1.38 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 19 | 1.38 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 19 | 1.38 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 15 | 1.38 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 15 | 1.38 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 20 | 1.38 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 20 | 1.38 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 20 | 1.38 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 7 | 1.38 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 2 | 1.38 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 2 | 1.38 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 2 | 1.38 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 2 | 1.38 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 2 | 1.38 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 2 | 1.38 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 2 | 1.38 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 2 | 1.38 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 2 | 1.38 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 20 | 1.38 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 20 | 1.38 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 20 | 1.38 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 6 | 1.38 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 6 | 1.38 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 6 | 1.38 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 1 | 1.38 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 13 | 1.38 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 13 | 1.38 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 13 | 1.38 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 17 | 1.38 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 17 | 1.38 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 17 | 1.38 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 15 | 1.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 15 | 1.38 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 15 | 1.38 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 15 | 1.38 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 15 | 1.38 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 15 | 1.38 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 15 | 1.38 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 15 | 1.38 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 15 | 1.38 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 10 | 1.38 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 10 | 1.38 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 10 | 1.38 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 6 | 1.38 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 6 | 1.38 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 6 | 1.38 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 7 | 1.38 |
| (1,2017) | 1:117:A:LYS:HD3 | 1:120:A:ASP:H | 9 | 1.38 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 9 | 1.38 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 7 | 1.38 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 4 | 1.38 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 4 | 1.38 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 4 | 1.38 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 15 | 1.38 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 15 | 1.38 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 15 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 3 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 3 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 3 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 3 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 3 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 3 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 6 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 6 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 6 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 6 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 6 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 6 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 7 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 7 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 7 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 7 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 7 | 1.38 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 7 | 1.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 16 | 1.38 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 16 | 1.38 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 16 | 1.38 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 8 | 1.38 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 8 | 1.38 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 8 | 1.38 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 10 | 1.38 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 10 | 1.38 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 10 | 1.38 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 12 | 1.38 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 12 | 1.38 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 12 | 1.38 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 4 | 1.38 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 4 | 1.38 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 4 | 1.38 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 2 | 1.37 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 2 | 1.37 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 2 | 1.37 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 18 | 1.37 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 18 | 1.37 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 18 | 1.37 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 17 | 1.37 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 17 | 1.37 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 17 | 1.37 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 17 | 1.37 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 17 | 1.37 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 17 | 1.37 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 10 | 1.37 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 10 | 1.37 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 10 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 10 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 10 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 10 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 10 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 10 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 10 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 10 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 10 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 10 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 14 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 14 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 14 | 1.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 14 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 14 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 14 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 14 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 14 | 1.37 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 14 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 13 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 13 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 13 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 13 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 13 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 13 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 13 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 13 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 13 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 14 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 14 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 14 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 14 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 14 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 14 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 14 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 14 | 1.37 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 14 | 1.37 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 18 | 1.37 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 18 | 1.37 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 18 | 1.37 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 5 | 1.37 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 5 | 1.37 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 5 | 1.37 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 4 | 1.37 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 4 | 1.37 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 4 | 1.37 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 20 | 1.37 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 20 | 1.37 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 20 | 1.37 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 17 | 1.37 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 15 | 1.37 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 15 | 1.37 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 15 | 1.37 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 1 | 1.37 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 1 | 1.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 1 | 1.37 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 11 | 1.37 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 19 | 1.37 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 19 | 1.37 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 19 | 1.37 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 19 | 1.37 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 19 | 1.37 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 19 | 1.37 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 19 | 1.37 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 19 | 1.37 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 19 | 1.37 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 13 | 1.37 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 13 | 1.37 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 13 | 1.37 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 14 | 1.37 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 14 | 1.37 |
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 14 | 1.37 |
| (1,2003) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD3 | 11 | 1.37 |
| (1,2003) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD3 | 11 | 1.37 |
| (1,2003) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD3 | 11 | 1.37 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 13 | 1.37 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 1 | 1.37 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 2 | 1.37 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 2 | 1.37 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 2 | 1.37 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 2 | 1.37 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 2 | 1.37 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 2 | 1.37 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 6 | 1.37 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 6 | 1.37 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 6 | 1.37 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 13 | 1.37 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 13 | 1.37 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 13 | 1.37 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 16 | 1.37 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 16 | 1.37 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 16 | 1.37 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 18 | 1.36 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 18 | 1.36 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 9 | 1.36 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 9 | 1.36 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 9 | 1.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 1 | 1.36 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 1 | 1.36 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 1 | 1.36 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 11 | 1.36 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 11 | 1.36 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 11 | 1.36 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 12 | 1.36 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 12 | 1.36 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 12 | 1.36 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 7 | 1.36 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 7 | 1.36 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 7 | 1.36 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 7 | 1.36 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 7 | 1.36 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 7 | 1.36 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 7 | 1.36 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 7 | 1.36 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 7 | 1.36 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 14 | 1.36 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 14 | 1.36 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 14 | 1.36 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 19 | 1.36 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 20 | 1.36 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 11 | 1.36 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 11 | 1.36 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 11 | 1.36 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 9 | 1.36 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 9 | 1.36 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 9 | 1.36 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 17 | 1.36 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 16 | 1.36 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 16 | 1.36 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 16 | 1.36 |
| (1,1790) | 1:56:A:MET:HG3 | 1:57:A:THR:H | 8 | 1.36 |
| (1,1672) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG2 | 20 | 1.36 |
| (1,1672) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG2 | 20 | 1.36 |
| (1,1672) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG2 | 20 | 1.36 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 5 | 1.36 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 5 | 1.36 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 5 | 1.36 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 19 | 1.36 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 19 | 1.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 19 | 1.36 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 5 | 1.36 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 5 | 1.36 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 5 | 1.36 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 8 | 1.35 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 8 | 1.35 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 8 | 1.35 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 8 | 1.35 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 8 | 1.35 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 8 | 1.35 |
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 6 | 1.35 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 6 | 1.35 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 1 | 1.35 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 1 | 1.35 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 1 | 1.35 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 1 | 1.35 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 1 | 1.35 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 1 | 1.35 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 9 | 1.35 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 9 | 1.35 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 9 | 1.35 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 9 | 1.35 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 9 | 1.35 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 9 | 1.35 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 16 | 1.35 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 16 | 1.35 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 16 | 1.35 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 16 | 1.35 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 16 | 1.35 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 16 | 1.35 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 16 | 1.35 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 16 | 1.35 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 16 | 1.35 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 3 | 1.35 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 3 | 1.35 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 3 | 1.35 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 3 | 1.35 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 3 | 1.35 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 3 | 1.35 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 3 | 1.35 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 3 | 1.35 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 3 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 11 | 1.35 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 11 | 1.35 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 11 | 1.35 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 13 | 1.35 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 13 | 1.35 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 13 | 1.35 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 8 | 1.35 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 8 | 1.35 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 8 | 1.35 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 12 | 1.35 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 12 | 1.35 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 12 | 1.35 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 20 | 1.35 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 20 | 1.35 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 20 | 1.35 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 15 | 1.35 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 15 | 1.35 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 15 | 1.35 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 15 | 1.35 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 15 | 1.35 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 15 | 1.35 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 15 | 1.35 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 15 | 1.35 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 15 | 1.35 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 16 | 1.35 |
| (1,1715) | 1:133:A:LEU:H | 1:136:A:GLN:HG2 | 14 | 1.35 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 16 | 1.35 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 16 | 1.35 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 16 | 1.35 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 18 | 1.35 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 18 | 1.35 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 18 | 1.35 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 18 | 1.35 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 18 | 1.35 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 18 | 1.35 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 4 | 1.35 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 3 | 1.35 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 3 | 1.35 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 3 | 1.35 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 3 | 1.35 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 5 | 1.35 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 5 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 5 | 1.35 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 13 | 1.35 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 13 | 1.35 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 13 | 1.35 |
| (1,3527) | 1:73:A:GLN:HG2 | 1:125:A:TRP:HZ2 | 13 | 1.34 |
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 4 | 1.34 |
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 9 | 1.34 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 6 | 1.34 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 6 | 1.34 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 6 | 1.34 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 6 | 1.34 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 6 | 1.34 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 6 | 1.34 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 2 | 1.34 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 2 | 1.34 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 2 | 1.34 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 15 | 1.34 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 13 | 1.34 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 13 | 1.34 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 13 | 1.34 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 15 | 1.34 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 15 | 1.34 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 15 | 1.34 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 15 | 1.34 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 15 | 1.34 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 15 | 1.34 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 15 | 1.34 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 15 | 1.34 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 15 | 1.34 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 10 | 1.34 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 10 | 1.34 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 10 | 1.34 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 20 | 1.34 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 20 | 1.34 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 20 | 1.34 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 20 | 1.34 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 20 | 1.34 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 20 | 1.34 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 2 | 1.34 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 2 | 1.34 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 2 | 1.34 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 19 | 1.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 19 | 1.34 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 19 | 1.34 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 11 | 1.34 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 13 | 1.34 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 13 | 1.34 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 13 | 1.34 |
| (1,2304) | 1:132:A:SER:HA | 1:136:A:GLN:HG2 | 4 | 1.34 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 3 | 1.34 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 3 | 1.34 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 3 | 1.34 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 3 | 1.34 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 3 | 1.34 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 3 | 1.34 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 3 | 1.34 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 3 | 1.34 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 3 | 1.34 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 4 | 1.34 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 17 | 1.34 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 17 | 1.34 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 17 | 1.34 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 16 | 1.34 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 16 | 1.34 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 16 | 1.34 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 11 | 1.34 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 11 | 1.34 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 11 | 1.34 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 11 | 1.34 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 11 | 1.34 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 11 | 1.34 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 4 | 1.34 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 4 | 1.34 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 4 | 1.34 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 13 | 1.34 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 13 | 1.34 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 13 | 1.34 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 14 | 1.34 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 14 | 1.34 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 14 | 1.34 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 19 | 1.34 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 19 | 1.34 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 19 | 1.34 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 9 | 1.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 9 | 1.34 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 9 | 1.34 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 11 | 1.34 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 11 | 1.34 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 11 | 1.34 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 2 | 1.34 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 2 | 1.34 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 2 | 1.34 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 3 | 1.33 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 3 | 1.33 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 3 | 1.33 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 3 | 1.33 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 3 | 1.33 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 3 | 1.33 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 7 | 1.33 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 7 | 1.33 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 7 | 1.33 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 7 | 1.33 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 7 | 1.33 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 7 | 1.33 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 15 | 1.33 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 15 | 1.33 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 15 | 1.33 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 15 | 1.33 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 15 | 1.33 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 15 | 1.33 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 12 | 1.33 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 12 | 1.33 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 12 | 1.33 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 10 | 1.33 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 10 | 1.33 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 10 | 1.33 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 17 | 1.33 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 17 | 1.33 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 17 | 1.33 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 19 | 1.33 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 19 | 1.33 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 19 | 1.33 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 17 | 1.33 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 17 | 1.33 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 17 | 1.33 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 14 | 1.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 14 | 1.33 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 14 | 1.33 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 19 | 1.33 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 19 | 1.33 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 19 | 1.33 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 15 | 1.33 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 17 | 1.33 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 17 | 1.33 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 17 | 1.33 |
| (1,1697) | 1:132:A:SER:HB2 | 1:136:A:GLN:HG2 | 20 | 1.33 |
| (1,1697) | 1:132:A:SER:HB3 | 1:136:A:GLN:HG2 | 20 | 1.33 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 8 | 1.33 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 8 | 1.33 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 8 | 1.33 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 9 | 1.33 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 9 | 1.33 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 9 | 1.33 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 17 | 1.33 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 17 | 1.33 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 17 | 1.33 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 2 | 1.33 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 2 | 1.33 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 2 | 1.33 |
| (1,1432) | 1:85:A:ASP:HB3 | 1:86:A:LYS:HG2 | 10 | 1.33 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 15 | 1.33 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 15 | 1.33 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 15 | 1.33 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 3 | 1.33 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 3 | 1.33 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 20 | 1.33 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 20 | 1.33 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 20 | 1.33 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 18 | 1.33 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 1 | 1.33 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 1 | 1.33 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 1 | 1.33 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 6 | 1.33 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 6 | 1.33 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 6 | 1.33 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 2 | 1.33 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 2 | 1.33 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 2 | 1.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 17 | 1.33 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 17 | 1.33 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 17 | 1.33 |
| (1,353) | 1:108:A:ARG:HG3 | 1:112:A:VAL:H | 9 | 1.33 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 8 | 1.33 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 8 | 1.33 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG11 | 3 | 1.32 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG12 | 3 | 1.32 |
| (1,3503) | 1:34:A:TYR:HE1 | 1:39:A:VAL:HG13 | 3 | 1.32 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG11 | 3 | 1.32 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG12 | 3 | 1.32 |
| (1,3503) | 1:34:A:TYR:HE2 | 1:39:A:VAL:HG13 | 3 | 1.32 |
| (1,3480) | 1:32:A:HIS:HD2 | 1:150:A:PRO:HG3 | 16 | 1.32 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 7 | 1.32 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 7 | 1.32 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB2 | 12 | 1.32 |
| (1,3479) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HB3 | 12 | 1.32 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 7 | 1.32 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 7 | 1.32 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 10 | 1.32 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 10 | 1.32 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 15 | 1.32 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 15 | 1.32 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 2 | 1.32 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 2 | 1.32 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 2 | 1.32 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 2 | 1.32 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 2 | 1.32 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 2 | 1.32 |
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 14 | 1.32 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 14 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 4 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 4 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 4 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 4 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 4 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 4 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 5 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 5 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 5 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 5 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 5 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 5 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 10 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 10 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 10 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 10 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 10 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 10 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 13 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 13 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 13 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 13 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 13 | 1.32 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 13 | 1.32 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 18 | 1.32 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 18 | 1.32 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 18 | 1.32 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 18 | 1.32 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 18 | 1.32 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 18 | 1.32 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 18 | 1.32 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 18 | 1.32 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 18 | 1.32 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 2 | 1.32 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 2 | 1.32 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 2 | 1.32 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 19 | 1.32 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 19 | 1.32 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 19 | 1.32 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 8 | 1.32 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 8 | 1.32 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 8 | 1.32 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 16 | 1.32 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 16 | 1.32 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 16 | 1.32 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 7 | 1.32 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 7 | 1.32 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 7 | 1.32 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 10 | 1.32 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 10 | 1.32 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 10 | 1.32 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 9 | 1.32 |
| (1,2304) | 1:132:A:SER:HA | 1:136:A:GLN:HG2 | 20 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 5 | 1.32 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 5 | 1.32 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 5 | 1.32 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 5 | 1.32 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 5 | 1.32 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 5 | 1.32 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 5 | 1.32 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 5 | 1.32 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 5 | 1.32 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 4 | 1.32 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 4 | 1.32 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 4 | 1.32 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 4 | 1.32 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 4 | 1.32 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 4 | 1.32 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 5 | 1.32 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 5 | 1.32 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 5 | 1.32 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 5 | 1.32 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 5 | 1.32 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 5 | 1.32 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 8 | 1.32 |
| (1,1578) | 1:118:A:GLY:H | 1:119:A:GLU:HG3 | 2 | 1.32 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 8 | 1.32 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 8 | 1.32 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 8 | 1.32 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 5 | 1.32 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 4 | 1.32 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 4 | 1.32 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 4 | 1.32 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 15 | 1.32 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 15 | 1.32 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 15 | 1.32 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG21 | 12 | 1.32 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG22 | 12 | 1.32 |
| (1,336) | 1:166:A:ASP:H | 1:172:A:VAL:HG23 | 12 | 1.32 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 5 | 1.32 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 5 | 1.32 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 5 | 1.32 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 10 | 1.32 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 10 | 1.32 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 10 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 20 | 1.31 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 20 | 1.31 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 20 | 1.31 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 20 | 1.31 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 20 | 1.31 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 20 | 1.31 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 11 | 1.31 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 11 | 1.31 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 11 | 1.31 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 11 | 1.31 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 11 | 1.31 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 11 | 1.31 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 6 | 1.31 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 11 | 1.31 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 11 | 1.31 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 11 | 1.31 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 11 | 1.31 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 11 | 1.31 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 11 | 1.31 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 11 | 1.31 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 11 | 1.31 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 11 | 1.31 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 11 | 1.31 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 11 | 1.31 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 11 | 1.31 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 3 | 1.31 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 3 | 1.31 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 3 | 1.31 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 13 | 1.31 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 13 | 1.31 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 13 | 1.31 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 19 | 1.31 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 19 | 1.31 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 19 | 1.31 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 19 | 1.31 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 19 | 1.31 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 19 | 1.31 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 19 | 1.31 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 19 | 1.31 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 19 | 1.31 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 17 | 1.31 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 17 | 1.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 14 | 1.31 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 14 | 1.31 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 14 | 1.31 |
| (1,1578) | 1:118:A:GLY:H | 1:119:A:GLU:HG3 | 1 | 1.31 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 3 | 1.31 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 7 | 1.31 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 7 | 1.31 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 7 | 1.31 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 1 | 1.31 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 1 | 1.31 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 1 | 1.31 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 12 | 1.31 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 12 | 1.31 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 12 | 1.31 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 4 | 1.31 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 4 | 1.31 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 4 | 1.31 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 9 | 1.31 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 9 | 1.31 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 9 | 1.31 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG21 | 15 | 1.31 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG22 | 15 | 1.31 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG23 | 15 | 1.31 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG21 | 15 | 1.31 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG22 | 15 | 1.31 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG23 | 15 | 1.31 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 16 | 1.31 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 10 | 1.31 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 10 | 1.31 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 10 | 1.31 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 6 | 1.31 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 6 | 1.31 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 6 | 1.31 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 11 | 1.31 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 11 | 1.31 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 11 | 1.31 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 14 | 1.31 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 14 | 1.31 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 14 | 1.31 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 10 | 1.31 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 10 | 1.31 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 10 | 1.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 20 | 1.31 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 20 | 1.31 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 20 | 1.31 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 14 | 1.31 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 14 | 1.31 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 14 | 1.31 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 12 | 1.31 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 12 | 1.31 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 12 | 1.31 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 3 | 1.31 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 3 | 1.31 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 3 | 1.31 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 3 | 1.31 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 9 | 1.31 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 3 | 1.31 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 3 | 1.31 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 3 | 1.31 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 6 | 1.31 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 6 | 1.31 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 6 | 1.31 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 9 | 1.31 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 9 | 1.31 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 9 | 1.31 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 11 | 1.31 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 11 | 1.31 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 11 | 1.31 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 17 | 1.31 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 17 | 1.31 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 17 | 1.31 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 19 | 1.3 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 19 | 1.3 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 19 | 1.3 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 10 | 1.3 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 10 | 1.3 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 10 | 1.3 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 10 | 1.3 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 10 | 1.3 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 10 | 1.3 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE1 | 20 | 1.3 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE2 | 20 | 1.3 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE3 | 20 | 1.3 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 16 | 1.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 10 | 1.3 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 3 | 1.3 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 3 | 1.3 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 3 | 1.3 |
| (1,2722) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HA | 4 | 1.3 |
| (1,2722) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HA | 4 | 1.3 |
| (1,2722) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HA | 4 | 1.3 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 19 | 1.3 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 19 | 1.3 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 19 | 1.3 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 1 | 1.3 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 1 | 1.3 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 1 | 1.3 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 3 | 1.3 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 3 | 1.3 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 3 | 1.3 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 15 | 1.3 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 15 | 1.3 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 15 | 1.3 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 1 | 1.3 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 1 | 1.3 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 1 | 1.3 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 12 | 1.3 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 12 | 1.3 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 12 | 1.3 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 9 | 1.3 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 16 | 1.3 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 16 | 1.3 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 16 | 1.3 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 14 | 1.3 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 14 | 1.3 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 14 | 1.3 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 14 | 1.3 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 14 | 1.3 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 14 | 1.3 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB2 | 16 | 1.3 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB2 | 16 | 1.3 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB2 | 16 | 1.3 |
| (1,2066) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HB3 | 16 | 1.3 |
| (1,2066) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HB3 | 16 | 1.3 |
| (1,2066) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HB3 | 16 | 1.3 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 18 | 1.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 18 | 1.3 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 7 | 1.3 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 7 | 1.3 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 7 | 1.3 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB2 | 9 | 1.3 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB3 | 9 | 1.3 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 16 | 1.3 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 16 | 1.3 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 16 | 1.3 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 12 | 1.3 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 12 | 1.3 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 12 | 1.3 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 20 | 1.3 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 20 | 1.3 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 20 | 1.3 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 8 | 1.3 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 4 | 1.3 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 4 | 1.3 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 4 | 1.3 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 20 | 1.3 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 20 | 1.3 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 20 | 1.3 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 7 | 1.3 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 8 | 1.29 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 8 | 1.29 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 8 | 1.29 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 8 | 1.29 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 8 | 1.29 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 8 | 1.29 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 8 | 1.29 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 8 | 1.29 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 8 | 1.29 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 10 | 1.29 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 10 | 1.29 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 10 | 1.29 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG11 | 18 | 1.29 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG12 | 18 | 1.29 |
| (1,2985) | 1:114:A:ALA:HB1 | 1:116:A:VAL:HG13 | 18 | 1.29 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG11 | 18 | 1.29 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG12 | 18 | 1.29 |
| (1,2985) | 1:114:A:ALA:HB2 | 1:116:A:VAL:HG13 | 18 | 1.29 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG11 | 18 | 1.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG12 | 18 | 1.29 |
| (1,2985) | 1:114:A:ALA:HB3 | 1:116:A:VAL:HG13 | 18 | 1.29 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 2 | 1.29 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 2 | 1.29 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 2 | 1.29 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 2 | 1.29 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 2 | 1.29 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 2 | 1.29 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 2 | 1.29 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 2 | 1.29 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 2 | 1.29 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 13 | 1.29 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 13 | 1.29 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 13 | 1.29 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 18 | 1.29 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 18 | 1.29 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 18 | 1.29 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 12 | 1.29 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 15 | 1.29 |
| (1,2562) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HA | 11 | 1.29 |
| (1,2562) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HA | 11 | 1.29 |
| (1,2562) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HA | 11 | 1.29 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 4 | 1.29 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 4 | 1.29 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 4 | 1.29 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 18 | 1.29 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 18 | 1.29 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 18 | 1.29 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 15 | 1.29 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 15 | 1.29 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 15 | 1.29 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 16 | 1.29 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 16 | 1.29 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 16 | 1.29 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 8 | 1.29 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 15 | 1.29 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 13 | 1.29 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 13 | 1.29 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 13 | 1.29 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 13 | 1.29 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 13 | 1.29 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 13 | 1.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 14 | 1.29 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 14 | 1.29 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 14 | 1.29 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 7 | 1.29 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 3 | 1.29 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 19 | 1.29 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 19 | 1.29 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 19 | 1.29 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 4 | 1.29 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 4 | 1.29 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 17 | 1.29 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 17 | 1.29 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 17 | 1.29 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 13 | 1.29 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 7 | 1.29 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 7 | 1.29 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 7 | 1.29 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 18 | 1.29 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 18 | 1.29 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 18 | 1.29 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 15 | 1.29 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 15 | 1.29 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 15 | 1.29 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 11 | 1.29 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 11 | 1.29 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 11 | 1.29 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 15 | 1.28 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 15 | 1.28 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 20 | 1.28 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 20 | 1.28 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 20 | 1.28 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 20 | 1.28 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 20 | 1.28 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 20 | 1.28 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 10 | 1.28 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 10 | 1.28 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 10 | 1.28 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 2 | 1.28 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 2 | 1.28 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 2 | 1.28 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 8 | 1.28 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 8 | 1.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 8 | 1.28 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 5 | 1.28 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 5 | 1.28 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 5 | 1.28 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 5 | 1.28 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 5 | 1.28 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 5 | 1.28 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 5 | 1.28 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 5 | 1.28 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 5 | 1.28 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 17 | 1.28 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 2 | 1.28 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 2 | 1.28 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 2 | 1.28 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 14 | 1.28 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 14 | 1.28 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 14 | 1.28 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 7 | 1.28 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 7 | 1.28 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 7 | 1.28 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 17 | 1.28 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 17 | 1.28 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 17 | 1.28 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 8 | 1.28 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 8 | 1.28 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 8 | 1.28 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 19 | 1.28 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 19 | 1.28 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 19 | 1.28 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 19 | 1.28 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 19 | 1.28 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 19 | 1.28 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 11 | 1.28 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 11 | 1.28 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 11 | 1.28 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 1 | 1.28 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 1 | 1.28 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 1 | 1.28 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 15 | 1.28 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 15 | 1.28 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 15 | 1.28 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 15 | 1.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 15 | 1.28 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 15 | 1.28 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 7 | 1.28 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 14 | 1.28 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 14 | 1.28 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 14 | 1.28 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 12 | 1.28 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 12 | 1.28 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 12 | 1.28 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 2 | 1.28 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 2 | 1.28 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 2 | 1.28 |
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 15 | 1.27 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 14 | 1.27 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 14 | 1.27 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 10 | 1.27 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 10 | 1.27 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 10 | 1.27 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 19 | 1.27 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 19 | 1.27 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 19 | 1.27 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 19 | 1.27 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 19 | 1.27 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 19 | 1.27 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 10 | 1.27 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 10 | 1.27 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 10 | 1.27 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 10 | 1.27 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 10 | 1.27 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 10 | 1.27 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 10 | 1.27 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 10 | 1.27 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 10 | 1.27 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 5 | 1.27 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 5 | 1.27 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 5 | 1.27 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 15 | 1.27 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 15 | 1.27 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 15 | 1.27 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 11 | 1.27 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 13 | 1.27 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 13 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 13 | 1.27 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 20 | 1.27 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 20 | 1.27 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 20 | 1.27 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 10 | 1.27 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 10 | 1.27 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 10 | 1.27 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 12 | 1.27 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD1 | 13 | 1.27 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD2 | 13 | 1.27 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 13 | 1.27 |
| (1,2017) | 1:117:A:LYS:HD3 | 1:120:A:ASP:H | 8 | 1.27 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 12 | 1.27 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 17 | 1.27 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 1 | 1.27 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 1 | 1.27 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 1 | 1.27 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 16 | 1.27 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 16 | 1.27 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 16 | 1.27 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 18 | 1.27 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 18 | 1.27 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 18 | 1.27 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 18 | 1.27 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 18 | 1.27 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 18 | 1.27 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 2 | 1.27 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 4 | 1.27 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 4 | 1.27 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 4 | 1.27 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 2 | 1.27 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 2 | 1.27 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 2 | 1.27 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 4 | 1.27 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 4 | 1.27 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 4 | 1.27 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 13 | 1.26 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 13 | 1.26 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 13 | 1.26 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 13 | 1.26 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 13 | 1.26 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 13 | 1.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 18 | 1.26 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 18 | 1.26 |
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 20 | 1.26 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 20 | 1.26 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 11 | 1.26 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 11 | 1.26 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 15 | 1.26 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 15 | 1.26 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 15 | 1.26 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 15 | 1.26 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 15 | 1.26 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 15 | 1.26 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE1 | 1 | 1.26 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE2 | 1 | 1.26 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE3 | 1 | 1.26 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE1 | 2 | 1.26 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE2 | 2 | 1.26 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE3 | 2 | 1.26 |
| (1,2990) | 1:123:A:ALA:HA | 1:126:A:ASN:HB3 | 6 | 1.26 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG11 | 18 | 1.26 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG12 | 18 | 1.26 |
| (1,2923) | 1:94:A:ALA:HB1 | 1:101:A:VAL:HG13 | 18 | 1.26 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG11 | 18 | 1.26 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG12 | 18 | 1.26 |
| (1,2923) | 1:94:A:ALA:HB2 | 1:101:A:VAL:HG13 | 18 | 1.26 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG11 | 18 | 1.26 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG12 | 18 | 1.26 |
| (1,2923) | 1:94:A:ALA:HB3 | 1:101:A:VAL:HG13 | 18 | 1.26 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 9 | 1.26 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 9 | 1.26 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 9 | 1.26 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 9 | 1.26 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 9 | 1.26 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 9 | 1.26 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 9 | 1.26 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 9 | 1.26 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 9 | 1.26 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 12 | 1.26 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 12 | 1.26 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 12 | 1.26 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 5 | 1.26 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 5 | 1.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 5 | 1.26 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 7 | 1.26 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 7 | 1.26 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 7 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 1 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 1 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 1 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 1 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 1 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 1 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 1 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 1 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 1 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 14 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 14 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 14 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 14 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 14 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 14 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 14 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 14 | 1.26 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 14 | 1.26 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 5 | 1.26 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 13 | 1.26 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 11 | 1.26 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 11 | 1.26 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 11 | 1.26 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 11 | 1.26 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 11 | 1.26 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 11 | 1.26 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 8 | 1.26 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 8 | 1.26 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 8 | 1.26 |
| (1,2017) | 1:117:A:LYS:HD3 | 1:120:A:ASP:H | 17 | 1.26 |
| (1,2017) | 1:117:A:LYS:HD3 | 1:120:A:ASP:H | 20 | 1.26 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 14 | 1.26 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 6 | 1.26 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 6 | 1.26 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 6 | 1.26 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 17 | 1.26 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 17 | 1.26 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 17 | 1.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 1 | 1.26 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 1 | 1.26 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 1 | 1.26 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 14 | 1.26 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 14 | 1.26 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 14 | 1.26 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 6 | 1.26 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 2 | 1.26 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 2 | 1.26 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 2 | 1.26 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 16 | 1.26 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 5 | 1.26 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 5 | 1.26 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 5 | 1.26 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 18 | 1.26 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 18 | 1.26 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 18 | 1.26 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 14 | 1.26 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 14 | 1.26 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 14 | 1.26 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 2 | 1.26 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 2 | 1.26 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 2 | 1.26 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 12 | 1.26 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 13 | 1.26 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 13 | 1.26 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 13 | 1.26 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 19 | 1.26 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 19 | 1.26 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 19 | 1.26 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 9 | 1.25 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 9 | 1.25 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 9 | 1.25 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 9 | 1.25 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 9 | 1.25 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 9 | 1.25 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 16 | 1.25 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 16 | 1.25 |
| (1,3480) | 1:32:A:HIS:HD2 | 1:150:A:PRO:HG3 | 2 | 1.25 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 6 | 1.25 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 2 | 1.25 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 2 | 1.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 2 | 1.25 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 2 | 1.25 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 2 | 1.25 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 2 | 1.25 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 10 | 1.25 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 10 | 1.25 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 20 | 1.25 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 20 | 1.25 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 12 | 1.25 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 12 | 1.25 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 12 | 1.25 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 12 | 1.25 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 12 | 1.25 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 12 | 1.25 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 3 | 1.25 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 3 | 1.25 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 3 | 1.25 |
| (1,2945) | 1:23:A:LEU:HD21 | 1:58:A:LYS:HA | 3 | 1.25 |
| (1,2945) | 1:23:A:LEU:HD22 | 1:58:A:LYS:HA | 3 | 1.25 |
| (1,2945) | 1:23:A:LEU:HD23 | 1:58:A:LYS:HA | 3 | 1.25 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 3 | 1.25 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 3 | 1.25 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 3 | 1.25 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 3 | 1.25 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 3 | 1.25 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 3 | 1.25 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 3 | 1.25 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 3 | 1.25 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 3 | 1.25 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 7 | 1.25 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 7 | 1.25 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 7 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 2 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 2 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 2 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 2 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 2 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 2 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 2 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 2 | 1.25 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 2 | 1.25 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 8 | 1.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 8 | 1.25 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 8 | 1.25 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 1 | 1.25 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 8 | 1.25 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 12 | 1.25 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 15 | 1.25 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 15 | 1.25 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 15 | 1.25 |
| (1,1715) | 1:133:A:LEU:H | 1:136:A:GLN:HG2 | 15 | 1.25 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 3 | 1.25 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 3 | 1.25 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 3 | 1.25 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 12 | 1.25 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 12 | 1.25 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 12 | 1.25 |
| (1,989) | 1:125:A:TRP:HE1 | 1:126:A:ASN:HD22 | 13 | 1.25 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 19 | 1.25 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 19 | 1.25 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 19 | 1.25 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 1 | 1.25 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 1 | 1.25 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 1 | 1.25 |
| (1,353) | 1:108:A:ARG:HG3 | 1:112:A:VAL:H | 2 | 1.25 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 15 | 1.25 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 15 | 1.25 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 15 | 1.25 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD11 | 8 | 1.25 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD12 | 8 | 1.25 |
| (1,131) | 1:153:A:TYR:H | 1:160:A:LEU:HD13 | 8 | 1.25 |
| (1,3527) | 1:73:A:GLN:HG2 | 1:125:A:TRP:HZ2 | 18 | 1.24 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 5 | 1.24 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 5 | 1.24 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 5 | 1.24 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 16 | 1.24 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 16 | 1.24 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 16 | 1.24 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 11 | 1.24 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 11 | 1.24 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 11 | 1.24 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 11 | 1.24 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 11 | 1.24 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 11 | 1.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 11 | 1.24 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 11 | 1.24 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 11 | 1.24 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 7 | 1.24 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 7 | 1.24 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 7 | 1.24 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 8 | 1.24 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 8 | 1.24 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 8 | 1.24 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 9 | 1.24 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 9 | 1.24 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 9 | 1.24 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 9 | 1.24 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 9 | 1.24 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 9 | 1.24 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 5 | 1.24 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 5 | 1.24 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 5 | 1.24 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 5 | 1.24 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 5 | 1.24 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 5 | 1.24 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 3 | 1.24 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 3 | 1.24 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 15 | 1.24 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 15 | 1.24 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 15 | 1.24 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 4 | 1.24 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 4 | 1.24 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 4 | 1.24 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 13 | 1.24 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 13 | 1.24 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 13 | 1.24 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 3 | 1.24 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 3 | 1.24 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 3 | 1.24 |
| (1,1427) | 1:143:A:ASP:HB2 | 1:145:A:GLN:HE22 | 14 | 1.24 |
| (1,1409) | 1:67:A:LEU:HB2 | 1:70:A:ASP:HB3 | 3 | 1.24 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 3 | 1.24 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 3 | 1.24 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 3 | 1.24 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 12 | 1.24 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 12 | 1.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 12 | 1.24 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 12 | 1.24 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 12 | 1.24 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 12 | 1.24 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 1 | 1.24 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 1 | 1.24 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 1 | 1.24 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 8 | 1.24 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 14 | 1.24 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 14 | 1.24 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 14 | 1.24 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 19 | 1.24 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 19 | 1.24 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 19 | 1.24 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 7 | 1.24 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 7 | 1.24 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 7 | 1.24 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 6 | 1.24 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 6 | 1.24 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 6 | 1.24 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 14 | 1.23 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 14 | 1.23 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 19 | 1.23 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 19 | 1.23 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 19 | 1.23 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 19 | 1.23 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 19 | 1.23 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 19 | 1.23 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 19 | 1.23 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 19 | 1.23 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 19 | 1.23 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 16 | 1.23 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 16 | 1.23 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 16 | 1.23 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 16 | 1.23 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 16 | 1.23 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 16 | 1.23 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 16 | 1.23 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 16 | 1.23 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 16 | 1.23 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 16 | 1.23 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 16 | 1.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 16 | 1.23 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 20 | 1.23 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 20 | 1.23 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 20 | 1.23 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG21 | 15 | 1.23 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG22 | 15 | 1.23 |
| (1,2405) | 1:29:A:TYR:HA | 1:95:A:VAL:HG23 | 15 | 1.23 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 12 | 1.23 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 12 | 1.23 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 12 | 1.23 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 12 | 1.23 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 12 | 1.23 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 12 | 1.23 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 16 | 1.23 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 16 | 1.23 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 16 | 1.23 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 16 | 1.23 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 16 | 1.23 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 16 | 1.23 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 11 | 1.23 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 11 | 1.23 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 11 | 1.23 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 20 | 1.23 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 20 | 1.23 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 20 | 1.23 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 1 | 1.23 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 1 | 1.23 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 1 | 1.23 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 10 | 1.23 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 5 | 1.23 |
| (1,1697) | 1:132:A:SER:HB2 | 1:136:A:GLN:HG2 | 16 | 1.23 |
| (1,1697) | 1:132:A:SER:HB3 | 1:136:A:GLN:HG2 | 16 | 1.23 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 16 | 1.23 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 16 | 1.23 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 16 | 1.23 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 9 | 1.23 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 19 | 1.23 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 19 | 1.23 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 19 | 1.23 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 1 | 1.23 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 1 | 1.23 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 1 | 1.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 11 | 1.23 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 11 | 1.23 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 11 | 1.23 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 20 | 1.23 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 20 | 1.23 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 20 | 1.23 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 18 | 1.23 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 13 | 1.23 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 10 | 1.23 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 10 | 1.23 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 10 | 1.23 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 9 | 1.23 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 9 | 1.23 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 9 | 1.23 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 14 | 1.23 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 14 | 1.23 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 14 | 1.23 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 1 | 1.22 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 1 | 1.22 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 1 | 1.22 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 12 | 1.22 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 12 | 1.22 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 12 | 1.22 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 12 | 1.22 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 12 | 1.22 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 12 | 1.22 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 12 | 1.22 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 12 | 1.22 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 12 | 1.22 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 10 | 1.22 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 10 | 1.22 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 10 | 1.22 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 4 | 1.22 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 4 | 1.22 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 4 | 1.22 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 9 | 1.22 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 9 | 1.22 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 9 | 1.22 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 3 | 1.22 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 3 | 1.22 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 3 | 1.22 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 13 | 1.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 13 | 1.22 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 13 | 1.22 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 18 | 1.22 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 4 | 1.22 |
| (1,2331) | 1:3:A:ILE:HA | 1:9:A:TYR:H | 18 | 1.22 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 13 | 1.22 |
| (1,1990) | 1:133:A:LEU:HB3 | 1:136:A:GLN:HB2 | 17 | 1.22 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 18 | 1.22 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 3 | 1.22 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 3 | 1.22 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 3 | 1.22 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 13 | 1.22 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 13 | 1.22 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 13 | 1.22 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 19 | 1.22 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 19 | 1.22 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 19 | 1.22 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 2 | 1.22 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 2 | 1.22 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 2 | 1.22 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 6 | 1.22 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 6 | 1.22 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 6 | 1.22 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 7 | 1.22 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 7 | 1.22 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 7 | 1.22 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 13 | 1.22 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 13 | 1.22 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 13 | 1.22 |
| (1,1351) | 1:179:A:ASP:HB2 | 1:183:A:GLN:HE21 | 11 | 1.22 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 17 | 1.22 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 14 | 1.22 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 10 | 1.22 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 10 | 1.22 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 10 | 1.22 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 15 | 1.22 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 15 | 1.22 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 15 | 1.22 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 14 | 1.22 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 14 | 1.22 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 14 | 1.22 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 14 | 1.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 14 | 1.22 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 14 | 1.22 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 1 | 1.22 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 16 | 1.22 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 5 | 1.22 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 5 | 1.22 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 5 | 1.22 |
| (1,310) | 1:78:A:ALA:H | 1:79:A:ILE:HG12 | 5 | 1.22 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 10 | 1.22 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 10 | 1.22 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 10 | 1.22 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG11 | 15 | 1.22 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG12 | 15 | 1.22 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG13 | 15 | 1.22 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 3 | 1.22 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 3 | 1.22 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 3 | 1.22 |
| (1,3480) | 1:32:A:HIS:HD2 | 1:150:A:PRO:HG3 | 8 | 1.21 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 15 | 1.21 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 15 | 1.21 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 15 | 1.21 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 15 | 1.21 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 15 | 1.21 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 15 | 1.21 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 15 | 1.21 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 15 | 1.21 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 15 | 1.21 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 7 | 1.21 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 7 | 1.21 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 7 | 1.21 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG11 | 6 | 1.21 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG12 | 6 | 1.21 |
| (1,2617) | 1:182:A:LYS:HA | 1:185:A:VAL:HG13 | 6 | 1.21 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 12 | 1.21 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 12 | 1.21 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 12 | 1.21 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 15 | 1.21 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 15 | 1.21 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 15 | 1.21 |
| (1,2441) | 1:119:A:GLU:HA | 1:122:A:ASP:HB3 | 2 | 1.21 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 5 | 1.21 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 5 | 1.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 5 | 1.21 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 5 | 1.21 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 5 | 1.21 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 5 | 1.21 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 5 | 1.21 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 5 | 1.21 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 5 | 1.21 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 16 | 1.21 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 16 | 1.21 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 16 | 1.21 |
| (1,2019) | 1:86:A:LYS:HD2 | 1:115:A:GLY:H | 3 | 1.21 |
| (1,1963) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HD2 | 16 | 1.21 |
| (1,1963) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HD3 | 16 | 1.21 |
| (1,1578) | 1:118:A:GLY:H | 1:119:A:GLU:HG3 | 16 | 1.21 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 18 | 1.21 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 18 | 1.21 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 18 | 1.21 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 20 | 1.21 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 20 | 1.21 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 20 | 1.21 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 14 | 1.21 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 16 | 1.21 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 16 | 1.21 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 20 | 1.21 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 1 | 1.21 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 1 | 1.21 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 1 | 1.21 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 6 | 1.21 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 6 | 1.21 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 6 | 1.21 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG11 | 1 | 1.21 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG12 | 1 | 1.21 |
| (1,1201) | 1:100:A:THR:H | 1:101:A:VAL:HG13 | 1 | 1.21 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 9 | 1.21 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 13 | 1.21 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 13 | 1.21 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 13 | 1.21 |
| (1,763) | 1:103:A:SER:HB2 | 1:106:A:ASP:H | 19 | 1.21 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 10 | 1.21 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 10 | 1.21 |
| (1,102) | 1:50:A:LEU:HD21 | 1:56:A:MET:H | 5 | 1.21 |
| (1,102) | 1:50:A:LEU:HD22 | 1:56:A:MET:H | 5 | 1.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,102) | 1:50:A:LEU:HD23 | 1:56:A:MET:H | 5 | 1.21 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 20 | 1.21 |
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 5 | 1.2 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 5 | 1.2 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 15 | 1.2 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 15 | 1.2 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 15 | 1.2 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 5 | 1.2 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 5 | 1.2 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 5 | 1.2 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 17 | 1.2 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 17 | 1.2 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 17 | 1.2 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG11 | 9 | 1.2 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG12 | 9 | 1.2 |
| (1,2517) | 1:108:A:ARG:HA | 1:112:A:VAL:HG13 | 9 | 1.2 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 2 | 1.2 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 2 | 1.2 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 2 | 1.2 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 16 | 1.2 |
| (1,2015) | 1:117:A:LYS:HB2 | 1:117:A:LYS:HD3 | 5 | 1.2 |
| (1,2015) | 1:117:A:LYS:HB2 | 1:117:A:LYS:HD3 | 16 | 1.2 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 16 | 1.2 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 16 | 1.2 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 16 | 1.2 |
| (1,1859) | 1:103:A:SER:HB2 | 1:104:A:VAL:HB | 19 | 1.2 |
| (1,1859) | 1:103:A:SER:HB2 | 1:104:A:VAL:HB | 20 | 1.2 |
| (1,1715) | 1:133:A:LEU:H | 1:136:A:GLN:HG2 | 10 | 1.2 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 5 | 1.2 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 5 | 1.2 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 5 | 1.2 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 16 | 1.2 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 16 | 1.2 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 16 | 1.2 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 13 | 1.2 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 13 | 1.2 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 13 | 1.2 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 18 | 1.2 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 18 | 1.2 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 18 | 1.2 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 2 | 1.2 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 2 | 1.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 2 | 1.2 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 3 | 1.2 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 3 | 1.2 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 3 | 1.2 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 11 | 1.2 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 11 | 1.2 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 11 | 1.2 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 10 | 1.2 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 10 | 1.2 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 10 | 1.2 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 7 | 1.2 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 7 | 1.2 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 7 | 1.2 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 6 | 1.2 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 6 | 1.2 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 6 | 1.2 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 11 | 1.2 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 11 | 1.2 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 11 | 1.2 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 19 | 1.2 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 19 | 1.2 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 19 | 1.2 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 11 | 1.2 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 11 | 1.2 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 11 | 1.2 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 14 | 1.19 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 14 | 1.19 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 14 | 1.19 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 2 | 1.19 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 2 | 1.19 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 2 | 1.19 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 2 | 1.19 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 2 | 1.19 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 2 | 1.19 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 10 | 1.19 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 20 | 1.19 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 20 | 1.19 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 20 | 1.19 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 4 | 1.19 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 4 | 1.19 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 4 | 1.19 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 7 | 1.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 7 | 1.19 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 7 | 1.19 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 6 | 1.19 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 17 | 1.19 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 17 | 1.19 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 17 | 1.19 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 10 | 1.19 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 11 | 1.19 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 11 | 1.19 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 11 | 1.19 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 11 | 1.19 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 11 | 1.19 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 11 | 1.19 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 5 | 1.19 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 5 | 1.19 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 5 | 1.19 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 2 | 1.19 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 11 | 1.19 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 11 | 1.19 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 11 | 1.19 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 11 | 1.19 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 11 | 1.19 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 11 | 1.19 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 11 | 1.19 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 11 | 1.19 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 11 | 1.19 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 2 | 1.19 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 2 | 1.19 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 2 | 1.19 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 2 | 1.19 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 2 | 1.19 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 2 | 1.19 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 6 | 1.19 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 6 | 1.19 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 6 | 1.19 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD1 | 5 | 1.19 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD2 | 5 | 1.19 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 19 | 1.19 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 19 | 1.19 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 5 | 1.19 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 4 | 1.19 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 4 | 1.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 4 | 1.19 |
| (1,1578) | 1:118:A:GLY:H | 1:119:A:GLU:HG3 | 15 | 1.19 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 20 | 1.19 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 20 | 1.19 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 20 | 1.19 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 5 | 1.19 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 5 | 1.19 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 5 | 1.19 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 9 | 1.19 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 9 | 1.19 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 13 | 1.19 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 8 | 1.18 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 8 | 1.18 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 8 | 1.18 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 8 | 1.18 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 14 | 1.18 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 14 | 1.18 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 14 | 1.18 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 14 | 1.18 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 14 | 1.18 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 14 | 1.18 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE1 | 4 | 1.18 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE2 | 4 | 1.18 |
| (1,3078) | 1:46:A:VAL:HG21 | 1:56:A:MET:HE3 | 4 | 1.18 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE1 | 4 | 1.18 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE2 | 4 | 1.18 |
| (1,3078) | 1:46:A:VAL:HG22 | 1:56:A:MET:HE3 | 4 | 1.18 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE1 | 4 | 1.18 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE2 | 4 | 1.18 |
| (1,3078) | 1:46:A:VAL:HG23 | 1:56:A:MET:HE3 | 4 | 1.18 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 16 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 7 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 7 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 7 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 7 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 7 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 7 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 7 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 7 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 7 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 15 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 15 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 15 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 15 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 15 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 15 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 15 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 15 | 1.18 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 15 | 1.18 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 11 | 1.18 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 11 | 1.18 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 11 | 1.18 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 4 | 1.18 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 20 | 1.18 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 20 | 1.18 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 20 | 1.18 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 5 | 1.18 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 5 | 1.18 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 5 | 1.18 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 8 | 1.18 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 8 | 1.18 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 8 | 1.18 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 12 | 1.18 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 12 | 1.18 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 12 | 1.18 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 20 | 1.18 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 20 | 1.18 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 20 | 1.18 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 6 | 1.18 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 8 | 1.18 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 15 | 1.18 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 15 | 1.18 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 15 | 1.18 |
| (1,1859) | 1:103:A:SER:HB2 | 1:104:A:VAL:HB | 11 | 1.18 |
| (1,1578) | 1:118:A:GLY:H | 1:119:A:GLU:HG3 | 5 | 1.18 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 9 | 1.18 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 9 | 1.18 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 9 | 1.18 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 14 | 1.18 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 14 | 1.18 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 14 | 1.18 |
| (1,1206) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE22 | 15 | 1.18 |
| (1,1206) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE22 | 15 | 1.18 |
| (1,1206) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE22 | 15 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 10 | 1.18 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 10 | 1.18 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 10 | 1.18 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 5 | 1.18 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 12 | 1.18 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 14 | 1.18 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 19 | 1.18 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 2 | 1.18 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 2 | 1.18 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 2 | 1.18 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 7 | 1.18 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 7 | 1.18 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 7 | 1.18 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 7 | 1.18 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 14 | 1.18 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 14 | 1.18 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 14 | 1.18 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 8 | 1.18 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 8 | 1.18 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 8 | 1.18 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 12 | 1.18 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 12 | 1.18 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 12 | 1.18 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 19 | 1.18 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 19 | 1.18 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 19 | 1.18 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 13 | 1.18 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 13 | 1.18 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 13 | 1.18 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 9 | 1.18 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 9 | 1.18 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 9 | 1.18 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 2 | 1.18 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 2 | 1.18 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 2 | 1.18 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 3 | 1.18 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 3 | 1.18 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 3 | 1.18 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 5 | 1.18 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 5 | 1.18 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 5 | 1.18 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 16 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 16 | 1.18 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 16 | 1.18 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 9 | 1.18 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 9 | 1.18 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 9 | 1.18 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 5 | 1.17 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 5 | 1.17 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 5 | 1.17 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 5 | 1.17 |
| (1,3480) | 1:32:A:HIS:HD2 | 1:150:A:PRO:HG3 | 20 | 1.17 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 20 | 1.17 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 20 | 1.17 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 20 | 1.17 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 20 | 1.17 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 20 | 1.17 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 20 | 1.17 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 20 | 1.17 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 20 | 1.17 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 20 | 1.17 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 6 | 1.17 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 6 | 1.17 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 6 | 1.17 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 3 | 1.17 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 3 | 1.17 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 3 | 1.17 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 19 | 1.17 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 19 | 1.17 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 19 | 1.17 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 20 | 1.17 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 20 | 1.17 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 20 | 1.17 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 3 | 1.17 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 3 | 1.17 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 3 | 1.17 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 1 | 1.17 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 9 | 1.17 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 1 | 1.17 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 1 | 1.17 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 1 | 1.17 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 1 | 1.17 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 1 | 1.17 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 1 | 1.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 6 | 1.17 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 6 | 1.17 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 6 | 1.17 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 6 | 1.17 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 6 | 1.17 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 6 | 1.17 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 7 | 1.17 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD1 | 14 | 1.17 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD2 | 14 | 1.17 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 7 | 1.17 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG12 | 6 | 1.17 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG13 | 6 | 1.17 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 5 | 1.17 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 5 | 1.17 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 5 | 1.17 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 9 | 1.17 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 9 | 1.17 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 5 | 1.17 |
| (1,1520) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB3 | 7 | 1.17 |
| (1,1520) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB3 | 7 | 1.17 |
| (1,1520) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB3 | 7 | 1.17 |
| (1,1141) | 1:126:A:ASN:H | 1:127:A:SER:HB3 | 7 | 1.17 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 17 | 1.17 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 17 | 1.17 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 17 | 1.17 |
| (1,991) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HD22 | 20 | 1.17 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 2 | 1.17 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 2 | 1.17 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 2 | 1.17 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 2 | 1.17 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 2 | 1.17 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 2 | 1.17 |
| (1,242) | 1:145:A:GLN:HE21 | 1:147:A:GLN:H | 7 | 1.17 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 19 | 1.17 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 19 | 1.17 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 19 | 1.17 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 6 | 1.17 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 6 | 1.17 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 6 | 1.17 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 20 | 1.16 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 20 | 1.16 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 4 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 4 | 1.16 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 4 | 1.16 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 5 | 1.16 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 5 | 1.16 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 10 | 1.16 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 10 | 1.16 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 20 | 1.16 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 20 | 1.16 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 20 | 1.16 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 20 | 1.16 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 20 | 1.16 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 20 | 1.16 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 3 | 1.16 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 19 | 1.16 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 19 | 1.16 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 19 | 1.16 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 19 | 1.16 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 19 | 1.16 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 19 | 1.16 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 19 | 1.16 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 19 | 1.16 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 19 | 1.16 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 4 | 1.16 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 4 | 1.16 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 4 | 1.16 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 4 | 1.16 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 4 | 1.16 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 4 | 1.16 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 4 | 1.16 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 4 | 1.16 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 4 | 1.16 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 9 | 1.16 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 9 | 1.16 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 10 | 1.16 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 10 | 1.16 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 10 | 1.16 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 16 | 1.16 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 16 | 1.16 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 16 | 1.16 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 17 | 1.16 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 17 | 1.16 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 17 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 19 | 1.16 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 19 | 1.16 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 19 | 1.16 |
| (1,1351) | 1:179:A:ASP:HB2 | 1:183:A:GLN:HE21 | 2 | 1.16 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 2 | 1.16 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 14 | 1.16 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 14 | 1.16 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 14 | 1.16 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 19 | 1.16 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 3 | 1.16 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 2 | 1.16 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 2 | 1.16 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 2 | 1.16 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 12 | 1.16 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 19 | 1.16 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 19 | 1.16 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 19 | 1.16 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 4 | 1.16 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 4 | 1.16 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 4 | 1.16 |
| (1,353) | 1:108:A:ARG:HG3 | 1:112:A:VAL:H | 17 | 1.16 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 1 | 1.16 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 1 | 1.16 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 1 | 1.16 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 19 | 1.16 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 19 | 1.16 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 12 | 1.16 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 12 | 1.16 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 12 | 1.16 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 12 | 1.15 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 14 | 1.15 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 14 | 1.15 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 14 | 1.15 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 20 | 1.15 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 20 | 1.15 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 20 | 1.15 |
| (1,2672) | 1:185:A:VAL:HG21 | 1:186:A:GLU:HA | 8 | 1.15 |
| (1,2672) | 1:185:A:VAL:HG22 | 1:186:A:GLU:HA | 8 | 1.15 |
| (1,2672) | 1:185:A:VAL:HG23 | 1:186:A:GLU:HA | 8 | 1.15 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 5 | 1.15 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 5 | 1.15 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 5 | 1.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 11 | 1.15 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 11 | 1.15 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 11 | 1.15 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 11 | 1.15 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 11 | 1.15 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 11 | 1.15 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 11 | 1.15 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 11 | 1.15 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 11 | 1.15 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 18 | 1.15 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 18 | 1.15 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 18 | 1.15 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 3 | 1.15 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 4 | 1.15 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 4 | 1.15 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 4 | 1.15 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 13 | 1.15 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 13 | 1.15 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 13 | 1.15 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 13 | 1.15 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 13 | 1.15 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 13 | 1.15 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 1 | 1.15 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 1 | 1.15 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 1 | 1.15 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 1 | 1.15 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 1 | 1.15 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 1 | 1.15 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 11 | 1.15 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 11 | 1.15 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 11 | 1.15 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 16 | 1.15 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 16 | 1.15 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 16 | 1.15 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 6 | 1.15 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 6 | 1.15 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 6 | 1.15 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 14 | 1.15 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 14 | 1.15 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 14 | 1.15 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 4 | 1.15 |
| (1,2304) | 1:132:A:SER:HA | 1:136:A:GLN:HG2 | 12 | 1.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 12 | 1.15 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 12 | 1.15 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 12 | 1.15 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 12 | 1.15 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 12 | 1.15 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 12 | 1.15 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 12 | 1.15 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 12 | 1.15 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 12 | 1.15 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 4 | 1.15 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 4 | 1.15 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 4 | 1.15 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 14 | 1.15 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 14 | 1.15 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 14 | 1.15 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 18 | 1.15 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 18 | 1.15 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 18 | 1.15 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 16 | 1.15 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 16 | 1.15 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 16 | 1.15 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 1 | 1.15 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 5 | 1.15 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 5 | 1.15 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 5 | 1.15 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 14 | 1.15 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 14 | 1.15 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 14 | 1.15 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 4 | 1.15 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 4 | 1.15 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 4 | 1.15 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 8 | 1.15 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 8 | 1.15 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 8 | 1.15 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 5 | 1.15 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 5 | 1.15 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 5 | 1.15 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 8 | 1.15 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 8 | 1.15 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 8 | 1.15 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 18 | 1.15 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 18 | 1.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 18 | 1.15 |
| (1,1432) | 1:85:A:ASP:HB3 | 1:86:A:LYS:HG2 | 8 | 1.15 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 16 | 1.15 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 16 | 1.15 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 16 | 1.15 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 2 | 1.15 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 2 | 1.15 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 2 | 1.15 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 19 | 1.15 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 19 | 1.15 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 19 | 1.15 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD21 | 1 | 1.15 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD22 | 1 | 1.15 |
| (1,1286) | 1:47:A:ARG:HD2 | 1:50:A:LEU:HD23 | 1 | 1.15 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD21 | 1 | 1.15 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD22 | 1 | 1.15 |
| (1,1286) | 1:47:A:ARG:HD3 | 1:50:A:LEU:HD23 | 1 | 1.15 |
| (1,1213) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE21 | 18 | 1.15 |
| (1,1213) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE21 | 18 | 1.15 |
| (1,1213) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE21 | 18 | 1.15 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 16 | 1.15 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 12 | 1.15 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 12 | 1.15 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 12 | 1.15 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 5 | 1.15 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 11 | 1.15 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 11 | 1.15 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 11 | 1.15 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 11 | 1.15 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 11 | 1.15 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 11 | 1.15 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 10 | 1.15 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 10 | 1.15 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 10 | 1.15 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 5 | 1.15 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 5 | 1.15 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 19 | 1.15 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 1 | 1.14 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 1 | 1.14 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 1 | 1.14 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 1 | 1.14 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 1 | 1.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 1 | 1.14 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 6 | 1.14 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 6 | 1.14 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 6 | 1.14 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 6 | 1.14 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 6 | 1.14 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 6 | 1.14 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 2 | 1.14 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 2 | 1.14 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 2 | 1.14 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 8 | 1.14 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 16 | 1.14 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 16 | 1.14 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 16 | 1.14 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 16 | 1.14 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 16 | 1.14 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 16 | 1.14 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 16 | 1.14 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 16 | 1.14 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 16 | 1.14 |
| (1,2510) | 1:8:A:GLN:HA | 1:161:A:ASN:HD22 | 16 | 1.14 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 2 | 1.14 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 2 | 1.14 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 2 | 1.14 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 2 | 1.14 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 5 | 1.14 |
| (1,2015) | 1:117:A:LYS:HB2 | 1:117:A:LYS:HD3 | 1 | 1.14 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 20 | 1.14 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 1 | 1.14 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 1 | 1.14 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 19 | 1.14 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 19 | 1.14 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 19 | 1.14 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 2 | 1.14 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 2 | 1.14 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 2 | 1.14 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 10 | 1.14 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 10 | 1.14 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 10 | 1.14 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 15 | 1.14 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 6 | 1.14 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 11 | 1.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 11 | 1.14 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 11 | 1.14 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 16 | 1.14 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 16 | 1.14 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 16 | 1.14 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 9 | 1.14 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 9 | 1.14 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 9 | 1.14 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 9 | 1.14 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 9 | 1.14 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 9 | 1.14 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 8 | 1.14 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 8 | 1.14 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 8 | 1.14 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 17 | 1.14 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 17 | 1.14 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 17 | 1.14 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 12 | 1.13 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 12 | 1.13 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 12 | 1.13 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 12 | 1.13 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 12 | 1.13 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 12 | 1.13 |
| (1,3442) | 1:73:A:GLN:HG2 | 1:125:A:TRP:HH2 | 16 | 1.13 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 2 | 1.13 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 2 | 1.13 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 2 | 1.13 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 2 | 1.13 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 2 | 1.13 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 2 | 1.13 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 2 | 1.13 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 2 | 1.13 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 2 | 1.13 |
| (1,2965) | 1:165:A:MET:HA | 1:176:A:GLN:HE21 | 3 | 1.13 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 15 | 1.13 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 15 | 1.13 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 15 | 1.13 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 17 | 1.13 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 17 | 1.13 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 17 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 4 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 4 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 4 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 4 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 4 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 4 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 4 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 4 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 4 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 20 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 20 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 20 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 20 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 20 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 20 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 20 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 20 | 1.13 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 20 | 1.13 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 3 | 1.13 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 3 | 1.13 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 3 | 1.13 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 18 | 1.13 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 18 | 1.13 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 18 | 1.13 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 3 | 1.13 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 3 | 1.13 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 3 | 1.13 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 12 | 1.13 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 12 | 1.13 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 12 | 1.13 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 4 | 1.13 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 7 | 1.13 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 7 | 1.13 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 7 | 1.13 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 6 | 1.13 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 6 | 1.13 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 6 | 1.13 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 17 | 1.13 |
| (1,1578) | 1:118:A:GLY:H | 1:119:A:GLU:HG3 | 10 | 1.13 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 17 | 1.13 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 19 | 1.13 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 19 | 1.13 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 19 | 1.13 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 14 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 14 | 1.13 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 14 | 1.13 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 14 | 1.13 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 14 | 1.13 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 14 | 1.13 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 16 | 1.13 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 15 | 1.13 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 15 | 1.13 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 15 | 1.13 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 18 | 1.13 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 18 | 1.13 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 18 | 1.13 |
| (1,1058) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HA | 12 | 1.13 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 3 | 1.13 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 3 | 1.13 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 3 | 1.13 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 4 | 1.13 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 4 | 1.13 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 4 | 1.13 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 13 | 1.13 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 13 | 1.13 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 13 | 1.13 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG11 | 7 | 1.13 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG12 | 7 | 1.13 |
| (1,804) | 1:180:A:THR:H | 1:181:A:VAL:HG13 | 7 | 1.13 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 4 | 1.13 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 4 | 1.13 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 4 | 1.13 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 12 | 1.13 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 12 | 1.13 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 12 | 1.13 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 8 | 1.13 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 8 | 1.13 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 8 | 1.13 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 13 | 1.13 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 13 | 1.13 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 13 | 1.13 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 13 | 1.13 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 13 | 1.13 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 13 | 1.13 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 16 | 1.13 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 16 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 16 | 1.13 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 20 | 1.13 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 20 | 1.13 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 20 | 1.13 |
| (1,128) | 1:12:A:LEU:HD11 | 1:159:A:GLN:H | 20 | 1.13 |
| (1,128) | 1:12:A:LEU:HD12 | 1:159:A:GLN:H | 20 | 1.13 |
| (1,128) | 1:12:A:LEU:HD13 | 1:159:A:GLN:H | 20 | 1.13 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 17 | 1.12 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 17 | 1.12 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 17 | 1.12 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 17 | 1.12 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 17 | 1.12 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 17 | 1.12 |
| (1,3415) | 1:59:A:TYR:HD1 | 1:137:A:GLN:HG3 | 6 | 1.12 |
| (1,3415) | 1:59:A:TYR:HD2 | 1:137:A:GLN:HG3 | 6 | 1.12 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 6 | 1.12 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 6 | 1.12 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 6 | 1.12 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 6 | 1.12 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 6 | 1.12 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 6 | 1.12 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 9 | 1.12 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 9 | 1.12 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 9 | 1.12 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 9 | 1.12 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 9 | 1.12 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 9 | 1.12 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 16 | 1.12 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 16 | 1.12 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 16 | 1.12 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 16 | 1.12 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 16 | 1.12 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 16 | 1.12 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 18 | 1.12 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 18 | 1.12 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 18 | 1.12 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 18 | 1.12 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 18 | 1.12 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 18 | 1.12 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 8 | 1.12 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 8 | 1.12 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 8 | 1.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 5 | 1.12 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 5 | 1.12 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 5 | 1.12 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 9 | 1.12 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 9 | 1.12 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 9 | 1.12 |
| (1,2945) | 1:23:A:LEU:HD21 | 1:58:A:LYS:HA | 20 | 1.12 |
| (1,2945) | 1:23:A:LEU:HD22 | 1:58:A:LYS:HA | 20 | 1.12 |
| (1,2945) | 1:23:A:LEU:HD23 | 1:58:A:LYS:HA | 20 | 1.12 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 10 | 1.12 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 10 | 1.12 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 10 | 1.12 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 6 | 1.12 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 6 | 1.12 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 6 | 1.12 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 14 | 1.12 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 14 | 1.12 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 14 | 1.12 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 13 | 1.12 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 13 | 1.12 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 13 | 1.12 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 20 | 1.12 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 13 | 1.12 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 13 | 1.12 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 13 | 1.12 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 13 | 1.12 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 13 | 1.12 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 13 | 1.12 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 13 | 1.12 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 13 | 1.12 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 13 | 1.12 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 2 | 1.12 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 2 | 1.12 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 2 | 1.12 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 6 | 1.12 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 6 | 1.12 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 6 | 1.12 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 9 | 1.12 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 9 | 1.12 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 9 | 1.12 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 11 | 1.12 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 11 | 1.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 11 | 1.12 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 18 | 1.12 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 18 | 1.12 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 18 | 1.12 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 2 | 1.12 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 2 | 1.12 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 2 | 1.12 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 11 | 1.12 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 11 | 1.12 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 11 | 1.12 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 1 | 1.12 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 17 | 1.12 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 17 | 1.12 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 17 | 1.12 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 5 | 1.12 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 15 | 1.12 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 5 | 1.12 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 5 | 1.12 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 5 | 1.12 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 7 | 1.12 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 13 | 1.12 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 13 | 1.12 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 13 | 1.12 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG11 | 8 | 1.12 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG12 | 8 | 1.12 |
| (1,920) | 1:37:A:GLU:H | 1:42:A:VAL:HG13 | 8 | 1.12 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 20 | 1.12 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 20 | 1.12 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 20 | 1.12 |
| (1,112) | 1:105:A:ALA:H | 1:106:A:ASP:HB3 | 2 | 1.12 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 20 | 1.12 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 20 | 1.12 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 20 | 1.12 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 10 | 1.12 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 10 | 1.12 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 10 | 1.12 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 5 | 1.11 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 5 | 1.11 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 5 | 1.11 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 5 | 1.11 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 5 | 1.11 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 5 | 1.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 10 | 1.11 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 10 | 1.11 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 10 | 1.11 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 10 | 1.11 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 10 | 1.11 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 10 | 1.11 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 10 | 1.11 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 13 | 1.11 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 13 | 1.11 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 13 | 1.11 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 12 | 1.11 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 12 | 1.11 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 14 | 1.11 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 14 | 1.11 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 14 | 1.11 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 14 | 1.11 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 14 | 1.11 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 14 | 1.11 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 3 | 1.11 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 3 | 1.11 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 3 | 1.11 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 3 | 1.11 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 3 | 1.11 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 3 | 1.11 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 15 | 1.11 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 15 | 1.11 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 15 | 1.11 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 15 | 1.11 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 15 | 1.11 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 15 | 1.11 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 15 | 1.11 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 15 | 1.11 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 15 | 1.11 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 5 | 1.11 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 5 | 1.11 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 5 | 1.11 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 5 | 1.11 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 5 | 1.11 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 5 | 1.11 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 5 | 1.11 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 5 | 1.11 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 5 | 1.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 13 | 1.11 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 13 | 1.11 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 13 | 1.11 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 9 | 1.11 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 9 | 1.11 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 9 | 1.11 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 6 | 1.11 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 6 | 1.11 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 6 | 1.11 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 6 | 1.11 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 6 | 1.11 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 6 | 1.11 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 6 | 1.11 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 6 | 1.11 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 6 | 1.11 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 11 | 1.11 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 11 | 1.11 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 11 | 1.11 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 3 | 1.11 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 3 | 1.11 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 3 | 1.11 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 3 | 1.11 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 3 | 1.11 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 3 | 1.11 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 1 | 1.11 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 1 | 1.11 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 1 | 1.11 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 10 | 1.11 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 10 | 1.11 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 10 | 1.11 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 13 | 1.11 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 13 | 1.11 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 13 | 1.11 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 17 | 1.11 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 17 | 1.11 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 17 | 1.11 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 17 | 1.11 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 17 | 1.11 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 17 | 1.11 |
| (1,2015) | 1:117:A:LYS:HB2 | 1:117:A:LYS:HD3 | 20 | 1.11 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 4 | 1.11 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 4 | 1.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 4 | 1.11 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 6 | 1.11 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 6 | 1.11 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 6 | 1.11 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 15 | 1.11 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 15 | 1.11 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 15 | 1.11 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 17 | 1.11 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 2 | 1.11 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 2 | 1.11 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 2 | 1.11 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 7 | 1.11 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 7 | 1.11 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 7 | 1.11 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 13 | 1.11 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 13 | 1.11 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 13 | 1.11 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 4 | 1.11 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 4 | 1.11 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 4 | 1.11 |
| (1,353) | 1:108:A:ARG:HG3 | 1:112:A:VAL:H | 15 | 1.11 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 18 | 1.11 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 18 | 1.11 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 18 | 1.11 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 17 | 1.11 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 17 | 1.11 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 17 | 1.11 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 11 | 1.1 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 11 | 1.1 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 11 | 1.1 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 11 | 1.1 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 11 | 1.1 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 11 | 1.1 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 9 | 1.1 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 9 | 1.1 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 10 | 1.1 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 10 | 1.1 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 10 | 1.1 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 10 | 1.1 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 10 | 1.1 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 10 | 1.1 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 8 | 1.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 8 | 1.1 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 8 | 1.1 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 8 | 1.1 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 8 | 1.1 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 8 | 1.1 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 19 | 1.1 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 19 | 1.1 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 19 | 1.1 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 3 | 1.1 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 3 | 1.1 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 3 | 1.1 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 8 | 1.1 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 8 | 1.1 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 8 | 1.1 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 7 | 1.1 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 7 | 1.1 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 7 | 1.1 |
| (1,2441) | 1:119:A:GLU:HA | 1:122:A:ASP:HB3 | 8 | 1.1 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 7 | 1.1 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 7 | 1.1 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 7 | 1.1 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 7 | 1.1 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 7 | 1.1 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 7 | 1.1 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 7 | 1.1 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 7 | 1.1 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 7 | 1.1 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 17 | 1.1 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 17 | 1.1 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 17 | 1.1 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 20 | 1.1 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 16 | 1.1 |
| (1,2304) | 1:132:A:SER:HA | 1:136:A:GLN:HG2 | 16 | 1.1 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 8 | 1.1 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 8 | 1.1 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 8 | 1.1 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 15 | 1.1 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 15 | 1.1 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 15 | 1.1 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 5 | 1.1 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 5 | 1.1 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 5 | 1.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 19 | 1.1 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 19 | 1.1 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 19 | 1.1 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 5 | 1.1 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 5 | 1.1 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 5 | 1.1 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 16 | 1.1 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 2 | 1.1 |
| (1,2015) | 1:117:A:LYS:HB2 | 1:117:A:LYS:HD3 | 18 | 1.1 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 11 | 1.1 |
| (1,1669) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HG2 | 8 | 1.1 |
| (1,1669) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HG2 | 8 | 1.1 |
| (1,1669) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HG2 | 8 | 1.1 |
| (1,1669) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HG2 | 9 | 1.1 |
| (1,1669) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HG2 | 9 | 1.1 |
| (1,1669) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HG2 | 9 | 1.1 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 15 | 1.1 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 5 | 1.1 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 5 | 1.1 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 5 | 1.1 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 19 | 1.1 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 9 | 1.1 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 9 | 1.1 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 9 | 1.1 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG21 | 11 | 1.1 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG22 | 11 | 1.1 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG23 | 11 | 1.1 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG21 | 11 | 1.1 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG22 | 11 | 1.1 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG23 | 11 | 1.1 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 15 | 1.1 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 12 | 1.1 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 1 | 1.1 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 1 | 1.1 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 1 | 1.1 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 8 | 1.1 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 18 | 1.1 |
| (1,1058) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HA | 20 | 1.1 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 8 | 1.1 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 8 | 1.1 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 8 | 1.1 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 9 | 1.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 9 | 1.1 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 9 | 1.1 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 19 | 1.1 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 19 | 1.1 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 19 | 1.1 |
| (1,763) | 1:103:A:SER:HB2 | 1:106:A:ASP:H | 20 | 1.1 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 8 | 1.1 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 8 | 1.1 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 8 | 1.1 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 13 | 1.1 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 13 | 1.1 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 6 | 1.09 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 6 | 1.09 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 6 | 1.09 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 6 | 1.09 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 6 | 1.09 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 6 | 1.09 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 10 | 1.09 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 10 | 1.09 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 5 | 1.09 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 11 | 1.09 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 11 | 1.09 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 11 | 1.09 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 11 | 1.09 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 11 | 1.09 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 11 | 1.09 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 15 | 1.09 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 19 | 1.09 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 10 | 1.09 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 10 | 1.09 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 10 | 1.09 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG11 | 2 | 1.09 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG12 | 2 | 1.09 |
| (1,2616) | 1:183:A:GLN:H | 1:185:A:VAL:HG13 | 2 | 1.09 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 7 | 1.09 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 7 | 1.09 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 7 | 1.09 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 13 | 1.09 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 13 | 1.09 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 13 | 1.09 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 3 | 1.09 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 5 | 1.09 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 5 | 1.09 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 5 | 1.09 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 19 | 1.09 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 19 | 1.09 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 19 | 1.09 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 20 | 1.09 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 20 | 1.09 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 20 | 1.09 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 18 | 1.09 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 18 | 1.09 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 18 | 1.09 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 18 | 1.09 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 18 | 1.09 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 18 | 1.09 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 19 | 1.09 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 19 | 1.09 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 19 | 1.09 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 2 | 1.09 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 2 | 1.09 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 19 | 1.09 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 19 | 1.09 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 19 | 1.09 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG12 | 18 | 1.09 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG13 | 18 | 1.09 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 7 | 1.09 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 20 | 1.09 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 14 | 1.09 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 14 | 1.09 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 14 | 1.09 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 8 | 1.09 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 8 | 1.09 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 8 | 1.09 |
| (1,1427) | 1:143:A:ASP:HB2 | 1:145:A:GLN:HE22 | 6 | 1.09 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG21 | 10 | 1.09 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG22 | 10 | 1.09 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG23 | 10 | 1.09 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG21 | 10 | 1.09 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG22 | 10 | 1.09 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG23 | 10 | 1.09 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 11 | 1.09 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 8 | 1.09 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 8 | 1.09 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 8 | 1.09 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 14 | 1.09 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 14 | 1.09 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 14 | 1.09 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 15 | 1.09 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 15 | 1.09 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 15 | 1.09 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 1 | 1.09 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 20 | 1.09 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 2 | 1.09 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 16 | 1.09 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 17 | 1.09 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 20 | 1.09 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 12 | 1.09 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 12 | 1.09 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 12 | 1.09 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 11 | 1.09 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 11 | 1.09 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 11 | 1.09 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 5 | 1.09 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 5 | 1.09 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 5 | 1.09 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 15 | 1.09 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 15 | 1.09 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 15 | 1.09 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 16 | 1.09 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 16 | 1.09 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 16 | 1.09 |
| (1,112) | 1:105:A:ALA:H | 1:106:A:ASP:HB3 | 9 | 1.09 |
| (1,102) | 1:50:A:LEU:HD21 | 1:56:A:MET:H | 19 | 1.09 |
| (1,102) | 1:50:A:LEU:HD22 | 1:56:A:MET:H | 19 | 1.09 |
| (1,102) | 1:50:A:LEU:HD23 | 1:56:A:MET:H | 19 | 1.09 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 9 | 1.09 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 9 | 1.09 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 9 | 1.09 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 8 | 1.08 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 8 | 1.08 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 8 | 1.08 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 8 | 1.08 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 8 | 1.08 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 8 | 1.08 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 8 | 1.08 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 8 | 1.08 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 19 | 1.08 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 4 | 1.08 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 4 | 1.08 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 4 | 1.08 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 4 | 1.08 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 4 | 1.08 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 4 | 1.08 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 4 | 1.08 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 4 | 1.08 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 4 | 1.08 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 4 | 1.08 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 4 | 1.08 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 4 | 1.08 |
| (1,3294) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA2 | 6 | 1.08 |
| (1,3294) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA2 | 6 | 1.08 |
| (1,3294) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA2 | 6 | 1.08 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 6 | 1.08 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 6 | 1.08 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 6 | 1.08 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 6 | 1.08 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 6 | 1.08 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 6 | 1.08 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 6 | 1.08 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 6 | 1.08 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 6 | 1.08 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 7 | 1.08 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 7 | 1.08 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 7 | 1.08 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 7 | 1.08 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 7 | 1.08 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 7 | 1.08 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 7 | 1.08 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 7 | 1.08 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 7 | 1.08 |
| (1,2945) | 1:23:A:LEU:HD21 | 1:58:A:LYS:HA | 11 | 1.08 |
| (1,2945) | 1:23:A:LEU:HD22 | 1:58:A:LYS:HA | 11 | 1.08 |
| (1,2945) | 1:23:A:LEU:HD23 | 1:58:A:LYS:HA | 11 | 1.08 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 6 | 1.08 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 6 | 1.08 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 6 | 1.08 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 6 | 1.08 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 6 | 1.08 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 6 | 1.08 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 6 | 1.08 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 6 | 1.08 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 6 | 1.08 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 2 | 1.08 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 2 | 1.08 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 2 | 1.08 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 14 | 1.08 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 14 | 1.08 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 14 | 1.08 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 12 | 1.08 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 12 | 1.08 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 12 | 1.08 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 6 | 1.08 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 6 | 1.08 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 6 | 1.08 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 19 | 1.08 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 19 | 1.08 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 19 | 1.08 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 9 | 1.08 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 9 | 1.08 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 9 | 1.08 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 14 | 1.08 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 14 | 1.08 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 14 | 1.08 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 6 | 1.08 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 10 | 1.08 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 9 | 1.08 |
| (1,2015) | 1:117:A:LYS:HB2 | 1:117:A:LYS:HD3 | 2 | 1.08 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 17 | 1.08 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 17 | 1.08 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 17 | 1.08 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 6 | 1.08 |
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 1 | 1.08 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 6 | 1.08 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 12 | 1.08 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 12 | 1.08 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 12 | 1.08 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB2 | 3 | 1.08 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB3 | 3 | 1.08 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 16 | 1.08 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 16 | 1.08 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 16 | 1.08 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 20 | 1.08 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 20 | 1.08 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 20 | 1.08 |
| (1,1509) | 1:16:A:ILE:HB | 1:156:A:GLY:HA3 | 3 | 1.08 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 4 | 1.08 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 5 | 1.08 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 5 | 1.08 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 5 | 1.08 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 19 | 1.08 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 19 | 1.08 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 19 | 1.08 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 4 | 1.08 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 4 | 1.08 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 9 | 1.08 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 17 | 1.08 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 17 | 1.08 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 17 | 1.08 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 3 | 1.08 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 3 | 1.08 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 3 | 1.08 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 3 | 1.08 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 3 | 1.08 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 3 | 1.08 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 17 | 1.08 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 17 | 1.08 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 17 | 1.08 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 2 | 1.08 |
| (1,353) | 1:108:A:ARG:HG3 | 1:112:A:VAL:H | 3 | 1.08 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 13 | 1.07 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 13 | 1.07 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 13 | 1.07 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 13 | 1.07 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 13 | 1.07 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 13 | 1.07 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 16 | 1.07 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 16 | 1.07 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 16 | 1.07 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 16 | 1.07 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 5 | 1.07 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 17 | 1.07 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 17 | 1.07 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 17 | 1.07 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 13 | 1.07 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 13 | 1.07 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 13 | 1.07 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 13 | 1.07 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 13 | 1.07 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 13 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 12 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 12 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 12 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 12 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 12 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 12 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 12 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 12 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 12 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 17 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 17 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 17 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 17 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 17 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 17 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 17 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 17 | 1.07 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 17 | 1.07 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 13 | 1.07 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 13 | 1.07 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 13 | 1.07 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 1 | 1.07 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 1 | 1.07 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 1 | 1.07 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 19 | 1.07 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 19 | 1.07 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 19 | 1.07 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG11 | 4 | 1.07 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG12 | 4 | 1.07 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG13 | 4 | 1.07 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 14 | 1.07 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 14 | 1.07 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 14 | 1.07 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 15 | 1.07 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 15 | 1.07 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 15 | 1.07 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 19 | 1.07 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 19 | 1.07 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 19 | 1.07 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 6 | 1.07 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 6 | 1.07 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 6 | 1.07 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 4 | 1.07 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 4 | 1.07 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 7 | 1.07 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 7 | 1.07 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 13 | 1.07 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 13 | 1.07 |
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 11 | 1.07 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 5 | 1.07 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 5 | 1.07 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 5 | 1.07 |
| (1,1669) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HG2 | 14 | 1.07 |
| (1,1669) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HG2 | 14 | 1.07 |
| (1,1669) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HG2 | 14 | 1.07 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 11 | 1.07 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 11 | 1.07 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 11 | 1.07 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 4 | 1.07 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 4 | 1.07 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 4 | 1.07 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 6 | 1.07 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 6 | 1.07 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 6 | 1.07 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 16 | 1.07 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 16 | 1.07 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 16 | 1.07 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 15 | 1.07 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG11 | 1 | 1.07 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG12 | 1 | 1.07 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG13 | 1 | 1.07 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 1 | 1.07 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 5 | 1.07 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 12 | 1.07 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 19 | 1.07 |
| (1,1058) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HA | 2 | 1.07 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 18 | 1.07 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 18 | 1.07 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 18 | 1.07 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD21 | 16 | 1.07 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD22 | 16 | 1.07 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD23 | 16 | 1.07 |
| (1,683) | 1:168:A:SER:H | 1:170:A:MET:HG2 | 19 | 1.07 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 10 | 1.07 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 10 | 1.07 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 10 | 1.07 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 15 | 1.06 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 15 | 1.06 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 15 | 1.06 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 15 | 1.06 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 15 | 1.06 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 15 | 1.06 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 13 | 1.06 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 13 | 1.06 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 14 | 1.06 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 14 | 1.06 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 11 | 1.06 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 11 | 1.06 |
| (1,3412) | 1:36:A:PHE:HD1 | 1:40:A:LEU:HD11 | 18 | 1.06 |
| (1,3412) | 1:36:A:PHE:HD1 | 1:40:A:LEU:HD12 | 18 | 1.06 |
| (1,3412) | 1:36:A:PHE:HD1 | 1:40:A:LEU:HD13 | 18 | 1.06 |
| (1,3412) | 1:36:A:PHE:HD2 | 1:40:A:LEU:HD11 | 18 | 1.06 |
| (1,3412) | 1:36:A:PHE:HD2 | 1:40:A:LEU:HD12 | 18 | 1.06 |
| (1,3412) | 1:36:A:PHE:HD2 | 1:40:A:LEU:HD13 | 18 | 1.06 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 11 | 1.06 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 11 | 1.06 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 11 | 1.06 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 11 | 1.06 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 11 | 1.06 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 11 | 1.06 |
| (1,3252) | 1:29:A:TYR:HD1 | 1:68:A:GLY:HA3 | 16 | 1.06 |
| (1,3252) | 1:29:A:TYR:HD2 | 1:68:A:GLY:HA3 | 16 | 1.06 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD11 | 8 | 1.06 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD12 | 8 | 1.06 |
| (1,2799) | 1:153:A:TYR:HA | 1:160:A:LEU:HD13 | 8 | 1.06 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 14 | 1.06 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 14 | 1.06 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 14 | 1.06 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 8 | 1.06 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 8 | 1.06 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 8 | 1.06 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 18 | 1.06 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 18 | 1.06 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 18 | 1.06 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 1 | 1.06 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 1 | 1.06 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 1 | 1.06 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 1 | 1.06 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 1 | 1.06 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 1 | 1.06 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 12 | 1.06 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 12 | 1.06 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 12 | 1.06 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 9 | 1.06 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 9 | 1.06 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 9 | 1.06 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 12 | 1.06 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 12 | 1.06 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 12 | 1.06 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 1 | 1.06 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 1 | 1.06 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 1 | 1.06 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 1 | 1.06 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 1 | 1.06 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 1 | 1.06 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 10 | 1.06 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 10 | 1.06 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 10 | 1.06 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 9 | 1.06 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 12 | 1.06 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 17 | 1.06 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 16 | 1.06 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 16 | 1.06 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 16 | 1.06 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 17 | 1.06 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 17 | 1.06 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 17 | 1.06 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 19 | 1.06 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 19 | 1.06 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 19 | 1.06 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 19 | 1.06 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 19 | 1.06 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 19 | 1.06 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 2 | 1.06 |
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 17 | 1.06 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 15 | 1.06 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 15 | 1.06 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 15 | 1.06 |
| (1,1578) | 1:118:A:GLY:H | 1:119:A:GLU:HG3 | 7 | 1.06 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG11 | 15 | 1.06 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG12 | 15 | 1.06 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG13 | 15 | 1.06 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 7 | 1.06 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 7 | 1.06 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 7 | 1.06 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 2 | 1.06 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 7 | 1.06 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 11 | 1.06 |
| (1,353) | 1:108:A:ARG:HG3 | 1:112:A:VAL:H | 1 | 1.06 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 8 | 1.06 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 8 | 1.06 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 8 | 1.06 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 18 | 1.06 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 5 | 1.05 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 5 | 1.05 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 9 | 1.05 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 9 | 1.05 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 12 | 1.05 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 8 | 1.05 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 6 | 1.05 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 6 | 1.05 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 6 | 1.05 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 5 | 1.05 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 5 | 1.05 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 5 | 1.05 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 5 | 1.05 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 5 | 1.05 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 5 | 1.05 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 7 | 1.05 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 7 | 1.05 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 7 | 1.05 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 7 | 1.05 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 7 | 1.05 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 7 | 1.05 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD11 | 10 | 1.05 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD12 | 10 | 1.05 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD13 | 10 | 1.05 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD11 | 10 | 1.05 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD12 | 10 | 1.05 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD13 | 10 | 1.05 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD11 | 16 | 1.05 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD12 | 16 | 1.05 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD13 | 16 | 1.05 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD11 | 16 | 1.05 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD12 | 16 | 1.05 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD13 | 16 | 1.05 |
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 8 | 1.05 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 8 | 1.05 |
| (1,3154) | 1:86:A:LYS:HD2 | 1:114:A:ALA:HA | 13 | 1.05 |
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 8 | 1.05 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 4 | 1.05 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 4 | 1.05 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 4 | 1.05 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 11 | 1.05 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 11 | 1.05 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 11 | 1.05 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 20 | 1.05 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 20 | 1.05 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 20 | 1.05 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 17 | 1.05 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 17 | 1.05 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 17 | 1.05 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 13 | 1.05 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 13 | 1.05 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 13 | 1.05 |
| (1,2392) | 1:31:A:PRO:HA | 1:34:A:TYR:HA | 14 | 1.05 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 5 | 1.05 |
| (1,2015) | 1:117:A:LYS:HB2 | 1:117:A:LYS:HD3 | 12 | 1.05 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 16 | 1.05 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 16 | 1.05 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 16 | 1.05 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 12 | 1.05 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 12 | 1.05 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 14 | 1.05 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 14 | 1.05 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 14 | 1.05 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 17 | 1.05 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 17 | 1.05 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 17 | 1.05 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 10 | 1.05 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 10 | 1.05 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 10 | 1.05 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 18 | 1.05 |
| (1,1573) | 1:119:A:GLU:HG2 | 1:120:A:ASP:HB2 | 8 | 1.05 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 16 | 1.05 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 16 | 1.05 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 16 | 1.05 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 6 | 1.05 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 6 | 1.05 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 6 | 1.05 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 10 | 1.05 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 10 | 1.05 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 10 | 1.05 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 2 | 1.05 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 2 | 1.05 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 2 | 1.05 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 2 | 1.05 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 2 | 1.05 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 2 | 1.05 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 9 | 1.05 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 9 | 1.05 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 9 | 1.05 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 6 | 1.05 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 14 | 1.05 |
| (1,1058) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HA | 17 | 1.05 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 3 | 1.05 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 3 | 1.05 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 3 | 1.05 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 13 | 1.05 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 13 | 1.05 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 13 | 1.05 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 15 | 1.05 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 15 | 1.05 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 15 | 1.05 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 18 | 1.05 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 18 | 1.05 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 18 | 1.05 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 4 | 1.05 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 4 | 1.05 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 4 | 1.05 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 18 | 1.05 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 18 | 1.05 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 18 | 1.05 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 7 | 1.05 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 7 | 1.05 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 7 | 1.05 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 12 | 1.05 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 12 | 1.05 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 12 | 1.05 |
| (1,112) | 1:105:A:ALA:H | 1:106:A:ASP:HB3 | 20 | 1.05 |
| (1,90) | 1:185:A:VAL:HA | 1:188:A:LYS:H | 20 | 1.05 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 13 | 1.04 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 19 | 1.04 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 19 | 1.04 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 19 | 1.04 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 19 | 1.04 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 19 | 1.04 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 19 | 1.04 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 8 | 1.04 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 8 | 1.04 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 8 | 1.04 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 8 | 1.04 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 8 | 1.04 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 8 | 1.04 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 20 | 1.04 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 20 | 1.04 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 20 | 1.04 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 2 | 1.04 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 7 | 1.04 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 5 | 1.04 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 5 | 1.04 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 5 | 1.04 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 6 | 1.04 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 6 | 1.04 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 6 | 1.04 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 9 | 1.04 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 9 | 1.04 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 9 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 9 | 1.04 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 9 | 1.04 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 9 | 1.04 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 9 | 1.04 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 9 | 1.04 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 9 | 1.04 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 14 | 1.04 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 14 | 1.04 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 14 | 1.04 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 14 | 1.04 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 14 | 1.04 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 14 | 1.04 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 14 | 1.04 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 14 | 1.04 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 14 | 1.04 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 11 | 1.04 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 11 | 1.04 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 11 | 1.04 |
| (1,2304) | 1:132:A:SER:HA | 1:136:A:GLN:HG2 | 5 | 1.04 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 2 | 1.04 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 2 | 1.04 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 2 | 1.04 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 2 | 1.04 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 2 | 1.04 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 2 | 1.04 |
| (1,2015) | 1:117:A:LYS:HB2 | 1:117:A:LYS:HD3 | 9 | 1.04 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 3 | 1.04 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 6 | 1.04 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 19 | 1.04 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 19 | 1.04 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 19 | 1.04 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 19 | 1.04 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 9 | 1.04 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 8 | 1.04 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 8 | 1.04 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 8 | 1.04 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 8 | 1.04 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 8 | 1.04 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 8 | 1.04 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 10 | 1.04 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 1 | 1.04 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 1 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 1 | 1.04 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 14 | 1.04 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 14 | 1.04 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 14 | 1.04 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 4 | 1.04 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 14 | 1.04 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 14 | 1.04 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 14 | 1.04 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 9 | 1.04 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 9 | 1.04 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 9 | 1.04 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 4 | 1.04 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 4 | 1.04 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 4 | 1.04 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 4 | 1.04 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 4 | 1.04 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 4 | 1.04 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 11 | 1.04 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 13 | 1.04 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 5 | 1.04 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 5 | 1.04 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 5 | 1.04 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 17 | 1.04 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 17 | 1.04 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 17 | 1.04 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 13 | 1.04 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 13 | 1.04 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 13 | 1.04 |
| (1,441) | 1:34:A:TYR:HE2 | 1:92:A:PHE:H | 14 | 1.04 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 18 | 1.04 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 18 | 1.04 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 18 | 1.04 |
| (1,112) | 1:105:A:ALA:H | 1:106:A:ASP:HB3 | 15 | 1.04 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG11 | 9 | 1.04 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG12 | 9 | 1.04 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG13 | 9 | 1.04 |
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 13 | 1.03 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 7 | 1.03 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 7 | 1.03 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 19 | 1.03 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 19 | 1.03 |
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG2 | 12 | 1.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3478) | 1:32:A:HIS:HD2 | 1:35:A:GLN:HG3 | 12 | 1.03 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 3 | 1.03 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 1 | 1.03 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 1 | 1.03 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 3 | 1.03 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 3 | 1.03 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 3 | 1.03 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 13 | 1.03 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 13 | 1.03 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 13 | 1.03 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 9 | 1.03 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 9 | 1.03 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 9 | 1.03 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 9 | 1.03 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 9 | 1.03 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 9 | 1.03 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 9 | 1.03 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 9 | 1.03 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 9 | 1.03 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 1 | 1.03 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 1 | 1.03 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 1 | 1.03 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 4 | 1.03 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 4 | 1.03 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 4 | 1.03 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 19 | 1.03 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 19 | 1.03 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 19 | 1.03 |
| (1,2392) | 1:31:A:PRO:HA | 1:34:A:TYR:HA | 13 | 1.03 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 15 | 1.03 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 15 | 1.03 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 15 | 1.03 |
| (1,2243) | 1:172:A:VAL:HG21 | 1:173:A:PHE:HA | 7 | 1.03 |
| (1,2243) | 1:172:A:VAL:HG22 | 1:173:A:PHE:HA | 7 | 1.03 |
| (1,2243) | 1:172:A:VAL:HG23 | 1:173:A:PHE:HA | 7 | 1.03 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 5 | 1.03 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 14 | 1.03 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 14 | 1.03 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 14 | 1.03 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 18 | 1.03 |
| (1,2017) | 1:117:A:LYS:HD3 | 1:120:A:ASP:H | 2 | 1.03 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 20 | 1.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 20 | 1.03 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 20 | 1.03 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 10 | 1.03 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 15 | 1.03 |
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 2 | 1.03 |
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 15 | 1.03 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 10 | 1.03 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 10 | 1.03 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 10 | 1.03 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 11 | 1.03 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 11 | 1.03 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 11 | 1.03 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 16 | 1.03 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 19 | 1.03 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 19 | 1.03 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 19 | 1.03 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 2 | 1.03 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 2 | 1.03 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 2 | 1.03 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 18 | 1.03 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 18 | 1.03 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 18 | 1.03 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 2 | 1.03 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 2 | 1.03 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 2 | 1.03 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 5 | 1.03 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 5 | 1.03 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 5 | 1.03 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 1 | 1.03 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 2 | 1.03 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 2 | 1.03 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 2 | 1.03 |
| (1,1262) | 1:29:A:TYR:HB3 | 1:64:A:LEU:HB2 | 1 | 1.03 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 9 | 1.03 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 9 | 1.03 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 9 | 1.03 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 15 | 1.03 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 15 | 1.03 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 15 | 1.03 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 19 | 1.03 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 19 | 1.03 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 19 | 1.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 6 | 1.03 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 6 | 1.03 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 6 | 1.03 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 1 | 1.03 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 1 | 1.03 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 1 | 1.03 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 5 | 1.03 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 5 | 1.03 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 5 | 1.03 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 15 | 1.03 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 15 | 1.03 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 15 | 1.03 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 17 | 1.03 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 17 | 1.03 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 17 | 1.03 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 4 | 1.03 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 4 | 1.03 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 4 | 1.03 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 2 | 1.03 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 14 | 1.03 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 14 | 1.03 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 14 | 1.03 |
| (1,112) | 1:105:A:ALA:H | 1:106:A:ASP:HB3 | 12 | 1.03 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 18 | 1.02 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 18 | 1.02 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 18 | 1.02 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 18 | 1.02 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 18 | 1.02 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 18 | 1.02 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 2 | 1.02 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 2 | 1.02 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 1 | 1.02 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 1 | 1.02 |
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 9 | 1.02 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 9 | 1.02 |
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 13 | 1.02 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 13 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 4 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 4 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 4 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 4 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 4 | 1.02 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 4 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 4 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 4 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 4 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 14 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 14 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 14 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 14 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 14 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 14 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 14 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 14 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 14 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 19 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 19 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 19 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 19 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 19 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 19 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 19 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 19 | 1.02 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 19 | 1.02 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 6 | 1.02 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 6 | 1.02 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 6 | 1.02 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 6 | 1.02 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 6 | 1.02 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 6 | 1.02 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 6 | 1.02 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 6 | 1.02 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 6 | 1.02 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG11 | 1 | 1.02 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG12 | 1 | 1.02 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG13 | 1 | 1.02 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 14 | 1.02 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 14 | 1.02 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 14 | 1.02 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 1 | 1.02 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 1 | 1.02 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 1 | 1.02 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 6 | 1.02 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 6 | 1.02 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 6 | 1.02 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 10 | 1.02 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 6 | 1.02 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 6 | 1.02 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 6 | 1.02 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 1 | 1.02 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 10 | 1.02 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 1 | 1.02 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 16 | 1.02 |
| (1,2210) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HA | 7 | 1.02 |
| (1,2210) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HA | 7 | 1.02 |
| (1,2210) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HA | 7 | 1.02 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 18 | 1.02 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 18 | 1.02 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 18 | 1.02 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 3 | 1.02 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 11 | 1.02 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 19 | 1.02 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 4 | 1.02 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 4 | 1.02 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 4 | 1.02 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 8 | 1.02 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 8 | 1.02 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 8 | 1.02 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 18 | 1.02 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 18 | 1.02 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 18 | 1.02 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 15 | 1.02 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 15 | 1.02 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 15 | 1.02 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 4 | 1.02 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 4 | 1.02 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 4 | 1.02 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 3 | 1.02 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 3 | 1.02 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 3 | 1.02 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 2 | 1.02 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 2 | 1.02 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 2 | 1.02 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 17 | 1.02 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 3 | 1.02 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 20 | 1.02 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 20 | 1.02 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 20 | 1.02 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 16 | 1.02 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 16 | 1.02 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 16 | 1.02 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 17 | 1.02 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 17 | 1.02 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 17 | 1.02 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 17 | 1.02 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 17 | 1.02 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 17 | 1.02 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 1 | 1.02 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 9 | 1.02 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 9 | 1.02 |
| (1,3480) | 1:32:A:HIS:HD2 | 1:150:A:PRO:HG3 | 9 | 1.01 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 19 | 1.01 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 14 | 1.01 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 14 | 1.01 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 14 | 1.01 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 14 | 1.01 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 14 | 1.01 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 14 | 1.01 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 17 | 1.01 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 17 | 1.01 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 17 | 1.01 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 17 | 1.01 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 17 | 1.01 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 17 | 1.01 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 3 | 1.01 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 3 | 1.01 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 3 | 1.01 |
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 15 | 1.01 |
| (1,2945) | 1:23:A:LEU:HD21 | 1:58:A:LYS:HA | 17 | 1.01 |
| (1,2945) | 1:23:A:LEU:HD22 | 1:58:A:LYS:HA | 17 | 1.01 |
| (1,2945) | 1:23:A:LEU:HD23 | 1:58:A:LYS:HA | 17 | 1.01 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 18 | 1.01 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 18 | 1.01 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 18 | 1.01 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 9 | 1.01 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 9 | 1.01 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 9 | 1.01 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 5 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 5 | 1.01 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 5 | 1.01 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 12 | 1.01 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 12 | 1.01 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 12 | 1.01 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 20 | 1.01 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 20 | 1.01 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 20 | 1.01 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 18 | 1.01 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 18 | 1.01 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 18 | 1.01 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 12 | 1.01 |
| (1,2015) | 1:117:A:LYS:HB2 | 1:117:A:LYS:HD3 | 17 | 1.01 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 18 | 1.01 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 6 | 1.01 |
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 8 | 1.01 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 1 | 1.01 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 1 | 1.01 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 1 | 1.01 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 1 | 1.01 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 9 | 1.01 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 9 | 1.01 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 9 | 1.01 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 19 | 1.01 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 19 | 1.01 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 19 | 1.01 |
| (1,1632) | 1:31:A:PRO:HA | 1:96:A:GLN:HG2 | 14 | 1.01 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 8 | 1.01 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 8 | 1.01 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 8 | 1.01 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 3 | 1.01 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 3 | 1.01 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 3 | 1.01 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 20 | 1.01 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 20 | 1.01 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 20 | 1.01 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 11 | 1.01 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 11 | 1.01 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 11 | 1.01 |
| (1,1141) | 1:126:A:ASN:H | 1:127:A:SER:HB3 | 6 | 1.01 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 10 | 1.01 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 7 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 7 | 1.01 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 7 | 1.01 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 5 | 1.01 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 5 | 1.01 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 5 | 1.01 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 12 | 1.01 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 12 | 1.01 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 12 | 1.01 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 12 | 1.01 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 12 | 1.01 |
| (1,112) | 1:105:A:ALA:H | 1:106:A:ASP:HB3 | 1 | 1.01 |
| (1,112) | 1:105:A:ALA:H | 1:106:A:ASP:HB3 | 18 | 1.01 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 12 | 1.01 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 19 | 1.0 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 19 | 1.0 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 15 | 1.0 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 20 | 1.0 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 20 | 1.0 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 20 | 1.0 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 15 | 1.0 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 15 | 1.0 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 15 | 1.0 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 15 | 1.0 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 15 | 1.0 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 15 | 1.0 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 5 | 1.0 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 16 | 1.0 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 16 | 1.0 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 16 | 1.0 |
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 10 | 1.0 |
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 7 | 1.0 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 11 | 1.0 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 11 | 1.0 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 11 | 1.0 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 14 | 1.0 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 14 | 1.0 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 14 | 1.0 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 9 | 1.0 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 9 | 1.0 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 9 | 1.0 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 3 | 1.0 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 3 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 3 | 1.0 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 9 | 1.0 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 9 | 1.0 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 9 | 1.0 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 19 | 1.0 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 19 | 1.0 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 19 | 1.0 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 11 | 1.0 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 11 | 1.0 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 11 | 1.0 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 9 | 1.0 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 9 | 1.0 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 9 | 1.0 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 1 | 1.0 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 1 | 1.0 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 1 | 1.0 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 1 | 1.0 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 1 | 1.0 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 1 | 1.0 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 1 | 1.0 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 1 | 1.0 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 1 | 1.0 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 7 | 1.0 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 7 | 1.0 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 7 | 1.0 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 11 | 1.0 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 10 | 1.0 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 10 | 1.0 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 10 | 1.0 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB2 | 3 | 1.0 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB3 | 3 | 1.0 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB2 | 5 | 1.0 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB3 | 5 | 1.0 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB2 | 17 | 1.0 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB3 | 17 | 1.0 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 8 | 1.0 |
| (1,2015) | 1:117:A:LYS:HB2 | 1:117:A:LYS:HD3 | 8 | 1.0 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 8 | 1.0 |
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 16 | 1.0 |
| (1,1697) | 1:132:A:SER:HB2 | 1:136:A:GLN:HG2 | 8 | 1.0 |
| (1,1697) | 1:132:A:SER:HB3 | 1:136:A:GLN:HG2 | 8 | 1.0 |
| (1,1641) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HB | 15 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1641) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HB | 15 | 1.0 |
| (1,1641) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HB | 15 | 1.0 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 16 | 1.0 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 2 | 1.0 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 2 | 1.0 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 2 | 1.0 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG21 | 7 | 1.0 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG22 | 7 | 1.0 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG23 | 7 | 1.0 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG21 | 7 | 1.0 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG22 | 7 | 1.0 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG23 | 7 | 1.0 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 18 | 1.0 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 1 | 1.0 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 1 | 1.0 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 1 | 1.0 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 20 | 1.0 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 20 | 1.0 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 20 | 1.0 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 19 | 1.0 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 19 | 1.0 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 19 | 1.0 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 14 | 1.0 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 14 | 1.0 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 17 | 1.0 |
| (1,112) | 1:105:A:ALA:H | 1:106:A:ASP:HB3 | 5 | 1.0 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 2 | 0.99 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 2 | 0.99 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 2 | 0.99 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 2 | 0.99 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 2 | 0.99 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 2 | 0.99 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 14 | 0.99 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 14 | 0.99 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 14 | 0.99 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 14 | 0.99 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 14 | 0.99 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 14 | 0.99 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 5 | 0.99 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 5 | 0.99 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE1 | 13 | 0.99 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE2 | 13 | 0.99 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 7 | 0.99 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 7 | 0.99 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 7 | 0.99 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 8 | 0.99 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 8 | 0.99 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 16 | 0.99 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 16 | 0.99 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 16 | 0.99 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 16 | 0.99 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 16 | 0.99 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 16 | 0.99 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 11 | 0.99 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 11 | 0.99 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 11 | 0.99 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 11 | 0.99 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 11 | 0.99 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 11 | 0.99 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 8 | 0.99 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 8 | 0.99 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 8 | 0.99 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 15 | 0.99 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 15 | 0.99 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 15 | 0.99 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 7 | 0.99 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 7 | 0.99 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 7 | 0.99 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 13 | 0.99 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 13 | 0.99 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 13 | 0.99 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 11 | 0.99 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 11 | 0.99 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 11 | 0.99 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 8 | 0.99 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 8 | 0.99 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 8 | 0.99 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 5 | 0.99 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 5 | 0.99 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 5 | 0.99 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 15 | 0.99 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 15 | 0.99 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 15 | 0.99 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 17 | 0.99 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 17 | 0.99 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 17 | 0.99 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 18 | 0.99 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 17 | 0.99 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 17 | 0.99 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 17 | 0.99 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB2 | 6 | 0.99 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB3 | 6 | 0.99 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 13 | 0.99 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 13 | 0.99 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 13 | 0.99 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 13 | 0.99 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 8 | 0.99 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 8 | 0.99 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 8 | 0.99 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 17 | 0.99 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 17 | 0.99 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 17 | 0.99 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 7 | 0.99 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 7 | 0.99 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 7 | 0.99 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 8 | 0.99 |
| (1,1375) | 1:8:A:GLN:HB3 | 1:9:A:TYR:HB2 | 19 | 0.99 |
| (1,1375) | 1:8:A:GLN:HB3 | 1:9:A:TYR:HB3 | 19 | 0.99 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 19 | 0.99 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 10 | 0.99 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 10 | 0.99 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 10 | 0.99 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 3 | 0.99 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 3 | 0.99 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 3 | 0.99 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 6 | 0.99 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 6 | 0.99 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 6 | 0.99 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 20 | 0.99 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 20 | 0.99 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 20 | 0.99 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 15 | 0.99 |
| (1,1058) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HA | 5 | 0.99 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 17 | 0.99 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 17 | 0.99 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 17 | 0.99 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 8 | 0.99 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 8 | 0.99 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 8 | 0.99 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 14 | 0.99 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 14 | 0.99 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 14 | 0.99 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 16 | 0.99 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 16 | 0.99 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 16 | 0.99 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 8 | 0.99 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 8 | 0.99 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 8 | 0.99 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 18 | 0.99 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 18 | 0.99 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 18 | 0.99 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 20 | 0.99 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 20 | 0.99 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 20 | 0.99 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 10 | 0.99 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 10 | 0.99 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 10 | 0.99 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 10 | 0.99 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 10 | 0.99 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 10 | 0.99 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 2 | 0.99 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 2 | 0.99 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 2 | 0.99 |
| (1,353) | 1:108:A:ARG:HG3 | 1:112:A:VAL:H | 13 | 0.99 |
| (1,90) | 1:185:A:VAL:HA | 1:188:A:LYS:H | 15 | 0.99 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 16 | 0.98 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 13 | 0.98 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 13 | 0.98 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 13 | 0.98 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 13 | 0.98 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 13 | 0.98 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 13 | 0.98 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 2 | 0.98 |
| (1,3269) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA2 | 15 | 0.98 |
| (1,3269) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA2 | 15 | 0.98 |
| (1,3269) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA2 | 15 | 0.98 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 15 | 0.98 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 15 | 0.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 15 | 0.98 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 20 | 0.98 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 20 | 0.98 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 20 | 0.98 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 20 | 0.98 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 20 | 0.98 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 20 | 0.98 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 20 | 0.98 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 20 | 0.98 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 20 | 0.98 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 3 | 0.98 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 3 | 0.98 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 3 | 0.98 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 8 | 0.98 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 8 | 0.98 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 8 | 0.98 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 12 | 0.98 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 12 | 0.98 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 12 | 0.98 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 10 | 0.98 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 10 | 0.98 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 10 | 0.98 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 15 | 0.98 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 15 | 0.98 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 15 | 0.98 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 9 | 0.98 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 9 | 0.98 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 9 | 0.98 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 18 | 0.98 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 18 | 0.98 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 18 | 0.98 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 14 | 0.98 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 14 | 0.98 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 14 | 0.98 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 15 | 0.98 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 3 | 0.98 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 20 | 0.98 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 20 | 0.98 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 20 | 0.98 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 20 | 0.98 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 20 | 0.98 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 20 | 0.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 20 | 0.98 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 20 | 0.98 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 20 | 0.98 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 7 | 0.98 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 7 | 0.98 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 7 | 0.98 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 7 | 0.98 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 7 | 0.98 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 7 | 0.98 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 7 | 0.98 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 7 | 0.98 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 7 | 0.98 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 11 | 0.98 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 18 | 0.98 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB2 | 10 | 0.98 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB3 | 10 | 0.98 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB2 | 10 | 0.98 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB3 | 10 | 0.98 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB2 | 10 | 0.98 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB3 | 10 | 0.98 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 9 | 0.98 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 9 | 0.98 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 9 | 0.98 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 9 | 0.98 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 9 | 0.98 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 9 | 0.98 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 3 | 0.98 |
| (1,1578) | 1:118:A:GLY:H | 1:119:A:GLU:HG3 | 11 | 0.98 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 8 | 0.98 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 14 | 0.98 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 14 | 0.98 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 14 | 0.98 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 7 | 0.98 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 7 | 0.98 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 7 | 0.98 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 19 | 0.98 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 9 | 0.98 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 9 | 0.98 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 9 | 0.98 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 12 | 0.98 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 12 | 0.98 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 12 | 0.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 18 | 0.98 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 18 | 0.98 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 18 | 0.98 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 20 | 0.98 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 20 | 0.98 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 20 | 0.98 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 15 | 0.98 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 15 | 0.98 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 15 | 0.98 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 6 | 0.98 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 6 | 0.98 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 6 | 0.98 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 2 | 0.98 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 2 | 0.98 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 2 | 0.98 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 1 | 0.97 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 1 | 0.97 |
| (1,3480) | 1:32:A:HIS:HD2 | 1:150:A:PRO:HG3 | 15 | 0.97 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 9 | 0.97 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 6 | 0.97 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 6 | 0.97 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 12 | 0.97 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 12 | 0.97 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 12 | 0.97 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 12 | 0.97 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 12 | 0.97 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 12 | 0.97 |
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 16 | 0.97 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 16 | 0.97 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 18 | 0.97 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 18 | 0.97 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 18 | 0.97 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 18 | 0.97 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 18 | 0.97 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 18 | 0.97 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 3 | 0.97 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 3 | 0.97 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 1 | 0.97 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 1 | 0.97 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 1 | 0.97 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 1 | 0.97 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 1 | 0.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 1 | 0.97 |
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 5 | 0.97 |
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 17 | 0.97 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG11 | 20 | 0.97 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG12 | 20 | 0.97 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG13 | 20 | 0.97 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 5 | 0.97 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 5 | 0.97 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 5 | 0.97 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 8 | 0.97 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 8 | 0.97 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 8 | 0.97 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 17 | 0.97 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 17 | 0.97 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 17 | 0.97 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 2 | 0.97 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 2 | 0.97 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 2 | 0.97 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 5 | 0.97 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 14 | 0.97 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 3 | 0.97 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 3 | 0.97 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 3 | 0.97 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 10 | 0.97 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 10 | 0.97 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 10 | 0.97 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 8 | 0.97 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 6 | 0.97 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 8 | 0.97 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 5 | 0.97 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 16 | 0.97 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 17 | 0.97 |
| (1,1859) | 1:103:A:SER:HB2 | 1:104:A:VAL:HB | 6 | 0.97 |
| (1,1807) | 1:179:A:ASP:HA | 1:182:A:LYS:HB3 | 17 | 0.97 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 9 | 0.97 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 20 | 0.97 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 20 | 0.97 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 20 | 0.97 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 12 | 0.97 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 5 | 0.97 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 5 | 0.97 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 5 | 0.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 5 | 0.97 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 12 | 0.97 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 12 | 0.97 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 12 | 0.97 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 15 | 0.97 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 2 | 0.97 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 17 | 0.97 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 17 | 0.97 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 17 | 0.97 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 11 | 0.97 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 6 | 0.97 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 6 | 0.97 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 6 | 0.97 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 6 | 0.97 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 6 | 0.97 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 6 | 0.97 |
| (1,112) | 1:105:A:ALA:H | 1:106:A:ASP:HB3 | 16 | 0.97 |
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 10 | 0.96 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 15 | 0.96 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 15 | 0.96 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 16 | 0.96 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 16 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 3 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 3 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 3 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 3 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 3 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 3 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 12 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 12 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 12 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 12 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 12 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 12 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 17 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 17 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 17 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 17 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 17 | 0.96 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 17 | 0.96 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 19 | 0.96 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 19 | 0.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 19 | 0.96 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 19 | 0.96 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 19 | 0.96 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 19 | 0.96 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 19 | 0.96 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 19 | 0.96 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 19 | 0.96 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 16 | 0.96 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 10 | 0.96 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 10 | 0.96 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 10 | 0.96 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE1 | 18 | 0.96 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE2 | 18 | 0.96 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE3 | 18 | 0.96 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 3 | 0.96 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 3 | 0.96 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 3 | 0.96 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 3 | 0.96 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 9 | 0.96 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 9 | 0.96 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 9 | 0.96 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 5 | 0.96 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 5 | 0.96 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 5 | 0.96 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 9 | 0.96 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 9 | 0.96 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 9 | 0.96 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 10 | 0.96 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 10 | 0.96 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 10 | 0.96 |
| (1,2558) | 1:40:A:LEU:HD21 | 1:170:A:MET:HB2 | 18 | 0.96 |
| (1,2558) | 1:40:A:LEU:HD22 | 1:170:A:MET:HB2 | 18 | 0.96 |
| (1,2558) | 1:40:A:LEU:HD23 | 1:170:A:MET:HB2 | 18 | 0.96 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 1 | 0.96 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 1 | 0.96 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 1 | 0.96 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 15 | 0.96 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 15 | 0.96 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 15 | 0.96 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 15 | 0.96 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 15 | 0.96 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 15 | 0.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 15 | 0.96 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 15 | 0.96 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 15 | 0.96 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 9 | 0.96 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 9 | 0.96 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 9 | 0.96 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 12 | 0.96 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 12 | 0.96 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 12 | 0.96 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 9 | 0.96 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 9 | 0.96 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 9 | 0.96 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 12 | 0.96 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 16 | 0.96 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 15 | 0.96 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 2 | 0.96 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 2 | 0.96 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 2 | 0.96 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 20 | 0.96 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 20 | 0.96 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 20 | 0.96 |
| (1,2015) | 1:117:A:LYS:HB2 | 1:117:A:LYS:HD3 | 14 | 0.96 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 7 | 0.96 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 10 | 0.96 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 12 | 0.96 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 15 | 0.96 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 20 | 0.96 |
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 20 | 0.96 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 13 | 0.96 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 13 | 0.96 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 13 | 0.96 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 13 | 0.96 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 8 | 0.96 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 12 | 0.96 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 12 | 0.96 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 12 | 0.96 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 7 | 0.96 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 7 | 0.96 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 7 | 0.96 |
| (1,1578) | 1:118:A:GLY:H | 1:119:A:GLU:HG3 | 18 | 0.96 |
| (1,1444) | 1:83:A:VAL:HA | 1:85:A:ASP:HB2 | 10 | 0.96 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 4 | 0.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 4 | 0.96 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 4 | 0.96 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG11 | 11 | 0.96 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG12 | 11 | 0.96 |
| (1,1434) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HG13 | 11 | 0.96 |
| (1,1377) | 1:144:A:LEU:HB2 | 1:145:A:GLN:HE22 | 9 | 0.96 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 2 | 0.96 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 2 | 0.96 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 2 | 0.96 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 10 | 0.96 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 10 | 0.96 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 10 | 0.96 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 14 | 0.96 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 1 | 0.96 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 1 | 0.96 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 1 | 0.96 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 7 | 0.96 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 7 | 0.96 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 7 | 0.96 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 15 | 0.96 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 15 | 0.96 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 15 | 0.96 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 20 | 0.96 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 20 | 0.96 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 20 | 0.96 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 13 | 0.96 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 1 | 0.96 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 1 | 0.96 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 1 | 0.96 |
| (1,353) | 1:108:A:ARG:HG3 | 1:112:A:VAL:H | 4 | 0.96 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 14 | 0.96 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 14 | 0.96 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 14 | 0.96 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 4 | 0.96 |
| (1,112) | 1:105:A:ALA:H | 1:106:A:ASP:HB3 | 19 | 0.96 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 16 | 0.96 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 20 | 0.95 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 20 | 0.95 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 20 | 0.95 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 20 | 0.95 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 18 | 0.95 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 18 | 0.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 17 | 0.95 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 17 | 0.95 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 5 | 0.95 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 5 | 0.95 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 5 | 0.95 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 5 | 0.95 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 5 | 0.95 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 5 | 0.95 |
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 3 | 0.95 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 3 | 0.95 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 5 | 0.95 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 5 | 0.95 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 5 | 0.95 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 5 | 0.95 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 5 | 0.95 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 5 | 0.95 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG21 | 14 | 0.95 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG22 | 14 | 0.95 |
| (1,3316) | 1:29:A:TYR:HD1 | 1:95:A:VAL:HG23 | 14 | 0.95 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG21 | 14 | 0.95 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG22 | 14 | 0.95 |
| (1,3316) | 1:29:A:TYR:HD2 | 1:95:A:VAL:HG23 | 14 | 0.95 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 2 | 0.95 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 2 | 0.95 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 2 | 0.95 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 8 | 0.95 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 8 | 0.95 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 8 | 0.95 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 6 | 0.95 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 6 | 0.95 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 6 | 0.95 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE1 | 1 | 0.95 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE2 | 1 | 0.95 |
| (1,2877) | 1:160:A:LEU:HD21 | 1:165:A:MET:HE3 | 1 | 0.95 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE1 | 1 | 0.95 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE2 | 1 | 0.95 |
| (1,2877) | 1:160:A:LEU:HD22 | 1:165:A:MET:HE3 | 1 | 0.95 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE1 | 1 | 0.95 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE2 | 1 | 0.95 |
| (1,2877) | 1:160:A:LEU:HD23 | 1:165:A:MET:HE3 | 1 | 0.95 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 18 | 0.95 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 18 | 0.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 18 | 0.95 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 17 | 0.95 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 17 | 0.95 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 17 | 0.95 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG11 | 17 | 0.95 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG12 | 17 | 0.95 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG13 | 17 | 0.95 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 1 | 0.95 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 1 | 0.95 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 1 | 0.95 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 19 | 0.95 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 19 | 0.95 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 19 | 0.95 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 19 | 0.95 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 19 | 0.95 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 19 | 0.95 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 19 | 0.95 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 19 | 0.95 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 19 | 0.95 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 16 | 0.95 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 16 | 0.95 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 16 | 0.95 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 15 | 0.95 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 19 | 0.95 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 19 | 0.95 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 19 | 0.95 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 15 | 0.95 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 11 | 0.95 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 11 | 0.95 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 11 | 0.95 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 8 | 0.95 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 1 | 0.95 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 13 | 0.95 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 19 | 0.95 |
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 12 | 0.95 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 13 | 0.95 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 13 | 0.95 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 13 | 0.95 |
| (1,1515) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HB2 | 7 | 0.95 |
| (1,1515) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HB2 | 7 | 0.95 |
| (1,1515) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HB2 | 7 | 0.95 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 4 | 0.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 4 | 0.95 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 4 | 0.95 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 4 | 0.95 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 4 | 0.95 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 4 | 0.95 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 1 | 0.95 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 1 | 0.95 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 1 | 0.95 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 12 | 0.95 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 20 | 0.95 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 20 | 0.95 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 20 | 0.95 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 1 | 0.95 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 1 | 0.95 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 1 | 0.95 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 2 | 0.95 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 2 | 0.95 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 2 | 0.95 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 15 | 0.95 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 15 | 0.95 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 15 | 0.95 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 15 | 0.95 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 15 | 0.95 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 15 | 0.95 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 4 | 0.95 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 4 | 0.95 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 4 | 0.95 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 8 | 0.95 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 8 | 0.95 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 8 | 0.95 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 14 | 0.95 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 2 | 0.95 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 2 | 0.95 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 2 | 0.95 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 14 | 0.95 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 14 | 0.95 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 14 | 0.95 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG21 | 13 | 0.95 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG22 | 13 | 0.95 |
| (1,552) | 1:46:A:VAL:H | 1:174:A:VAL:HG23 | 13 | 0.95 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 9 | 0.95 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 9 | 0.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 9 | 0.95 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 7 | 0.95 |
| (1,242) | 1:145:A:GLN:HE21 | 1:147:A:GLN:H | 6 | 0.95 |
| (1,163) | 1:69:A:LYS:H | 1:70:A:ASP:HB3 | 1 | 0.95 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 5 | 0.95 |
| (1,102) | 1:50:A:LEU:HD21 | 1:56:A:MET:H | 7 | 0.95 |
| (1,102) | 1:50:A:LEU:HD22 | 1:56:A:MET:H | 7 | 0.95 |
| (1,102) | 1:50:A:LEU:HD23 | 1:56:A:MET:H | 7 | 0.95 |
| (1,90) | 1:185:A:VAL:HA | 1:188:A:LYS:H | 3 | 0.95 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 20 | 0.94 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 20 | 0.94 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 9 | 0.94 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 9 | 0.94 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 9 | 0.94 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 9 | 0.94 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 5 | 0.94 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 19 | 0.94 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 2 | 0.94 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 2 | 0.94 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 2 | 0.94 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 2 | 0.94 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 2 | 0.94 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 2 | 0.94 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 17 | 0.94 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 17 | 0.94 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 17 | 0.94 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 17 | 0.94 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 17 | 0.94 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 17 | 0.94 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 18 | 0.94 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 20 | 0.94 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 20 | 0.94 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 20 | 0.94 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 6 | 0.94 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 6 | 0.94 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 6 | 0.94 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 6 | 0.94 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 6 | 0.94 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 6 | 0.94 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 6 | 0.94 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 6 | 0.94 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 6 | 0.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 17 | 0.94 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 20 | 0.94 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 20 | 0.94 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 20 | 0.94 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 3 | 0.94 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 3 | 0.94 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 3 | 0.94 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 10 | 0.94 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 10 | 0.94 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 10 | 0.94 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 4 | 0.94 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 4 | 0.94 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 4 | 0.94 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 6 | 0.94 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 6 | 0.94 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 6 | 0.94 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 14 | 0.94 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 14 | 0.94 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 14 | 0.94 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 18 | 0.94 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 18 | 0.94 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 18 | 0.94 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 13 | 0.94 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 13 | 0.94 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 13 | 0.94 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 20 | 0.94 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 20 | 0.94 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 20 | 0.94 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 7 | 0.94 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 7 | 0.94 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 7 | 0.94 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 6 | 0.94 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 15 | 0.94 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 1 | 0.94 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 1 | 0.94 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 1 | 0.94 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 15 | 0.94 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 6 | 0.94 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 11 | 0.94 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 18 | 0.94 |
| (1,2016) | 1:117:A:LYS:HD3 | 1:119:A:GLU:H | 17 | 0.94 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 13 | 0.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 13 | 0.94 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 13 | 0.94 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 3 | 0.94 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 15 | 0.94 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 15 | 0.94 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 15 | 0.94 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 7 | 0.94 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 7 | 0.94 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 7 | 0.94 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 16 | 0.94 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 16 | 0.94 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 16 | 0.94 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG11 | 8 | 0.94 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG12 | 8 | 0.94 |
| (1,1401) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HG13 | 8 | 0.94 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 18 | 0.94 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 6 | 0.94 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 6 | 0.94 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 6 | 0.94 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 3 | 0.94 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 3 | 0.94 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 3 | 0.94 |
| (1,1262) | 1:29:A:TYR:HB3 | 1:64:A:LEU:HB2 | 16 | 0.94 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG11 | 11 | 0.94 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG12 | 11 | 0.94 |
| (1,1103) | 1:41:A:HIS:H | 1:42:A:VAL:HG13 | 11 | 0.94 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG11 | 7 | 0.94 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG12 | 7 | 0.94 |
| (1,964) | 1:108:A:ARG:HE | 1:112:A:VAL:HG13 | 7 | 0.94 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 7 | 0.94 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 11 | 0.94 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 4 | 0.94 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 4 | 0.94 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 4 | 0.94 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 17 | 0.94 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 8 | 0.94 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 8 | 0.94 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 8 | 0.94 |
| (1,353) | 1:108:A:ARG:HG3 | 1:112:A:VAL:H | 12 | 0.94 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 20 | 0.94 |
| (1,112) | 1:105:A:ALA:H | 1:106:A:ASP:HB3 | 4 | 0.94 |
| (1,90) | 1:185:A:VAL:HA | 1:188:A:LYS:H | 4 | 0.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 14 | 0.94 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 15 | 0.94 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 3 | 0.93 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 3 | 0.93 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 3 | 0.93 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 3 | 0.93 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 3 | 0.93 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 3 | 0.93 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 4 | 0.93 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 4 | 0.93 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 4 | 0.93 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 4 | 0.93 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 4 | 0.93 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 4 | 0.93 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 18 | 0.93 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 18 | 0.93 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 5 | 0.93 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 5 | 0.93 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 5 | 0.93 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 15 | 0.93 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 15 | 0.93 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 15 | 0.93 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 15 | 0.93 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 15 | 0.93 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 15 | 0.93 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 5 | 0.93 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 5 | 0.93 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 7 | 0.93 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 7 | 0.93 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 7 | 0.93 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 7 | 0.93 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 7 | 0.93 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 7 | 0.93 |
| (1,3297) | 1:23:A:LEU:HB2 | 1:153:A:TYR:H | 18 | 0.93 |
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 18 | 0.93 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 18 | 0.93 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 18 | 0.93 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 6 | 0.93 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 6 | 0.93 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 6 | 0.93 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 15 | 0.93 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 15 | 0.93 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 15 | 0.93 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 8 | 0.93 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 8 | 0.93 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 8 | 0.93 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 15 | 0.93 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 15 | 0.93 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 15 | 0.93 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 17 | 0.93 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 17 | 0.93 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 17 | 0.93 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 3 | 0.93 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 3 | 0.93 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 3 | 0.93 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 5 | 0.93 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 5 | 0.93 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 5 | 0.93 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 5 | 0.93 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 5 | 0.93 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 5 | 0.93 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 11 | 0.93 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 11 | 0.93 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 11 | 0.93 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 13 | 0.93 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 8 | 0.93 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 8 | 0.93 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 8 | 0.93 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 8 | 0.93 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 8 | 0.93 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 8 | 0.93 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 6 | 0.93 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 6 | 0.93 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 6 | 0.93 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 6 | 0.93 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 6 | 0.93 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 6 | 0.93 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 3 | 0.93 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 11 | 0.93 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 11 | 0.93 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 11 | 0.93 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 17 | 0.93 |
| (1,2006) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HD2 | 8 | 0.93 |
| (1,2006) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HD2 | 8 | 0.93 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2006) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HD2 | 8 | 0.93 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 18 | 0.93 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 18 | 0.93 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 18 | 0.93 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 10 | 0.93 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 10 | 0.93 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 10 | 0.93 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 1 | 0.93 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 16 | 0.93 |
| (1,1697) | 1:132:A:SER:HB2 | 1:136:A:GLN:HG2 | 12 | 0.93 |
| (1,1697) | 1:132:A:SER:HB3 | 1:136:A:GLN:HG2 | 12 | 0.93 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 10 | 0.93 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 10 | 0.93 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 10 | 0.93 |
| (1,1427) | 1:143:A:ASP:HB2 | 1:145:A:GLN:HE22 | 11 | 0.93 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 16 | 0.93 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 19 | 0.93 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 19 | 0.93 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 19 | 0.93 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG11 | 5 | 0.93 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG12 | 5 | 0.93 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG13 | 5 | 0.93 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 3 | 0.93 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 3 | 0.93 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 3 | 0.93 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 10 | 0.93 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 10 | 0.93 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 10 | 0.93 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 17 | 0.93 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 17 | 0.93 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 17 | 0.93 |
| (1,778) | 1:51:A:PRO:HB3 | 1:54:A:THR:H | 20 | 0.93 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 6 | 0.93 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 6 | 0.93 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 6 | 0.93 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 12 | 0.93 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 12 | 0.93 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 12 | 0.93 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 18 | 0.93 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 2 | 0.93 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 2 | 0.93 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 2 | 0.93 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 11 | 0.93 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 11 | 0.93 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 11 | 0.93 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG21 | 8 | 0.93 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG22 | 8 | 0.93 |
| (1,406) | 1:25:A:PHE:H | 1:149:A:VAL:HG23 | 8 | 0.93 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 18 | 0.93 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 18 | 0.93 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 18 | 0.93 |
| (1,128) | 1:12:A:LEU:HD11 | 1:159:A:GLN:H | 6 | 0.93 |
| (1,128) | 1:12:A:LEU:HD12 | 1:159:A:GLN:H | 6 | 0.93 |
| (1,128) | 1:12:A:LEU:HD13 | 1:159:A:GLN:H | 6 | 0.93 |
| (1,112) | 1:105:A:ALA:H | 1:106:A:ASP:HB3 | 6 | 0.93 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 7 | 0.92 |
| (1,3351) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HB3 | 2 | 0.92 |
| (1,3351) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HB3 | 2 | 0.92 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 12 | 0.92 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 12 | 0.92 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 12 | 0.92 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 12 | 0.92 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 12 | 0.92 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 12 | 0.92 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 4 | 0.92 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 4 | 0.92 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 4 | 0.92 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 12 | 0.92 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 12 | 0.92 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 12 | 0.92 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 13 | 0.92 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 13 | 0.92 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 13 | 0.92 |
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 17 | 0.92 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 17 | 0.92 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 17 | 0.92 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 17 | 0.92 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 17 | 0.92 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 17 | 0.92 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG11 | 5 | 0.92 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG12 | 5 | 0.92 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG13 | 5 | 0.92 |
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 19 | 0.92 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD11 | 11 | 0.92 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD12 | 11 | 0.92 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD13 | 11 | 0.92 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 19 | 0.92 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 19 | 0.92 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 19 | 0.92 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 10 | 0.92 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 10 | 0.92 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 10 | 0.92 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 19 | 0.92 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 19 | 0.92 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 19 | 0.92 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 18 | 0.92 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 18 | 0.92 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 18 | 0.92 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 7 | 0.92 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 7 | 0.92 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 7 | 0.92 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG11 | 10 | 0.92 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG12 | 10 | 0.92 |
| (1,2457) | 1:43:A:SER:HB2 | 1:46:A:VAL:HG13 | 10 | 0.92 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG11 | 10 | 0.92 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG12 | 10 | 0.92 |
| (1,2457) | 1:43:A:SER:HB3 | 1:46:A:VAL:HG13 | 10 | 0.92 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 10 | 0.92 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 10 | 0.92 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 10 | 0.92 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 13 | 0.92 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 13 | 0.92 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 13 | 0.92 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 1 | 0.92 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 2 | 0.92 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 8 | 0.92 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 3 | 0.92 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 3 | 0.92 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 3 | 0.92 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 3 | 0.92 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 3 | 0.92 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 3 | 0.92 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 5 | 0.92 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 5 | 0.92 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 5 | 0.92 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 5 | 0.92 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 5 | 0.92 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 5 | 0.92 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 12 | 0.92 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 12 | 0.92 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 12 | 0.92 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 12 | 0.92 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 12 | 0.92 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 12 | 0.92 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 18 | 0.92 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 18 | 0.92 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 18 | 0.92 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 2 | 0.92 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 2 | 0.92 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 2 | 0.92 |
| (1,1697) | 1:132:A:SER:HB2 | 1:136:A:GLN:HG2 | 4 | 0.92 |
| (1,1697) | 1:132:A:SER:HB3 | 1:136:A:GLN:HG2 | 4 | 0.92 |
| (1,1657) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HG3 | 20 | 0.92 |
| (1,1657) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HG3 | 20 | 0.92 |
| (1,1657) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HG3 | 20 | 0.92 |
| (1,1632) | 1:31:A:PRO:HA | 1:96:A:GLN:HG2 | 7 | 0.92 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 7 | 0.92 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 7 | 0.92 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 7 | 0.92 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 7 | 0.92 |
| (1,1426) | 1:143:A:ASP:HB2 | 1:144:A:LEU:HG | 8 | 0.92 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 3 | 0.92 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 3 | 0.92 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 3 | 0.92 |
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 9 | 0.92 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 9 | 0.92 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 9 | 0.92 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 18 | 0.92 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 18 | 0.92 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 18 | 0.92 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD21 | 19 | 0.92 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD22 | 19 | 0.92 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD23 | 19 | 0.92 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 8 | 0.92 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 15 | 0.92 |
| (1,686) | 1:133:A:LEU:HD11 | 1:136:A:GLN:H | 18 | 0.92 |
| (1,686) | 1:133:A:LEU:HD12 | 1:136:A:GLN:H | 18 | 0.92 |
| (1,686) | 1:133:A:LEU:HD13 | 1:136:A:GLN:H | 18 | 0.92 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 3 | 0.92 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 3 | 0.92 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 3 | 0.92 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 12 | 0.92 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 12 | 0.92 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 12 | 0.92 |
| (1,163) | 1:69:A:LYS:H | 1:70:A:ASP:HB3 | 14 | 0.92 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 17 | 0.91 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 17 | 0.91 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 18 | 0.91 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 18 | 0.91 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 18 | 0.91 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 18 | 0.91 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 4 | 0.91 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 4 | 0.91 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 12 | 0.91 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 12 | 0.91 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE1 | 6 | 0.91 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE2 | 6 | 0.91 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 13 | 0.91 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 13 | 0.91 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 19 | 0.91 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 19 | 0.91 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 19 | 0.91 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 19 | 0.91 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 19 | 0.91 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 19 | 0.91 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 1 | 0.91 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 1 | 0.91 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 1 | 0.91 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 1 | 0.91 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 1 | 0.91 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 1 | 0.91 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 9 | 0.91 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 12 | 0.91 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 12 | 0.91 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 12 | 0.91 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 1 | 0.91 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 1 | 0.91 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 1 | 0.91 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 5 | 0.91 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 5 | 0.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 5 | 0.91 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG11 | 19 | 0.91 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG12 | 19 | 0.91 |
| (1,2679) | 1:109:A:LYS:HA | 1:112:A:VAL:HG13 | 19 | 0.91 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 16 | 0.91 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 8 | 0.91 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 8 | 0.91 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 8 | 0.91 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 20 | 0.91 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 20 | 0.91 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 20 | 0.91 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 5 | 0.91 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 5 | 0.91 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 5 | 0.91 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 18 | 0.91 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 18 | 0.91 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 18 | 0.91 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 4 | 0.91 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 4 | 0.91 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 4 | 0.91 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 13 | 0.91 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 13 | 0.91 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 13 | 0.91 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 3 | 0.91 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 3 | 0.91 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 3 | 0.91 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 10 | 0.91 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 10 | 0.91 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 10 | 0.91 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 11 | 0.91 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 2 | 0.91 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 17 | 0.91 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 15 | 0.91 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG11 | 9 | 0.91 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG12 | 9 | 0.91 |
| (1,2298) | 1:40:A:LEU:HD11 | 1:42:A:VAL:HG13 | 9 | 0.91 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG11 | 9 | 0.91 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG12 | 9 | 0.91 |
| (1,2298) | 1:40:A:LEU:HD12 | 1:42:A:VAL:HG13 | 9 | 0.91 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG11 | 9 | 0.91 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG12 | 9 | 0.91 |
| (1,2298) | 1:40:A:LEU:HD13 | 1:42:A:VAL:HG13 | 9 | 0.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 18 | 0.91 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 2 | 0.91 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 10 | 0.91 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 10 | 0.91 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 10 | 0.91 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 4 | 0.91 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 4 | 0.91 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 4 | 0.91 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 8 | 0.91 |
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 9 | 0.91 |
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 10 | 0.91 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 13 | 0.91 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 13 | 0.91 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 13 | 0.91 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 3 | 0.91 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 3 | 0.91 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 3 | 0.91 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 11 | 0.91 |
| (1,1577) | 1:152:A:MET:HB3 | 1:160:A:LEU:HB2 | 12 | 0.91 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 1 | 0.91 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 16 | 0.91 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 16 | 0.91 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 16 | 0.91 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 1 | 0.91 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 1 | 0.91 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 1 | 0.91 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 6 | 0.91 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 6 | 0.91 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 6 | 0.91 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 6 | 0.91 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 6 | 0.91 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 6 | 0.91 |
| (1,1358) | 1:179:A:ASP:HB3 | 1:183:A:GLN:HE21 | 3 | 0.91 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 5 | 0.91 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 5 | 0.91 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 5 | 0.91 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 9 | 0.91 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 9 | 0.91 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 9 | 0.91 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 18 | 0.91 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 18 | 0.91 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 18 | 0.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,416) | 1:122:A:ASP:HB3 | 1:123:A:ALA:H | 13 | 0.91 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 7 | 0.91 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 7 | 0.91 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 7 | 0.91 |
| (1,163) | 1:69:A:LYS:H | 1:70:A:ASP:HB3 | 5 | 0.91 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 13 | 0.91 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 2 | 0.91 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 2 | 0.91 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 2 | 0.91 |
| (1,102) | 1:50:A:LEU:HD21 | 1:56:A:MET:H | 15 | 0.91 |
| (1,102) | 1:50:A:LEU:HD22 | 1:56:A:MET:H | 15 | 0.91 |
| (1,102) | 1:50:A:LEU:HD23 | 1:56:A:MET:H | 15 | 0.91 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 7 | 0.91 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 20 | 0.91 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 20 | 0.91 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 20 | 0.91 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 19 | 0.9 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 19 | 0.9 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 20 | 0.9 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 20 | 0.9 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 20 | 0.9 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 20 | 0.9 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 20 | 0.9 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 20 | 0.9 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 20 | 0.9 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 20 | 0.9 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 14 | 0.9 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 14 | 0.9 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 15 | 0.9 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 15 | 0.9 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 15 | 0.9 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 17 | 0.9 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 17 | 0.9 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 17 | 0.9 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 15 | 0.9 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 15 | 0.9 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 15 | 0.9 |
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 12 | 0.9 |
| (1,2945) | 1:23:A:LEU:HD21 | 1:58:A:LYS:HA | 16 | 0.9 |
| (1,2945) | 1:23:A:LEU:HD22 | 1:58:A:LYS:HA | 16 | 0.9 |
| (1,2945) | 1:23:A:LEU:HD23 | 1:58:A:LYS:HA | 16 | 0.9 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 12 | 0.9 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 2 | 0.9 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 2 | 0.9 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 2 | 0.9 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 13 | 0.9 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 13 | 0.9 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 13 | 0.9 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 14 | 0.9 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 14 | 0.9 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 14 | 0.9 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG11 | 16 | 0.9 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG12 | 16 | 0.9 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG13 | 16 | 0.9 |
| (1,2553) | 1:40:A:LEU:HA | 1:40:A:LEU:HD21 | 18 | 0.9 |
| (1,2553) | 1:40:A:LEU:HA | 1:40:A:LEU:HD22 | 18 | 0.9 |
| (1,2553) | 1:40:A:LEU:HA | 1:40:A:LEU:HD23 | 18 | 0.9 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 1 | 0.9 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 1 | 0.9 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 1 | 0.9 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 1 | 0.9 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 1 | 0.9 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 1 | 0.9 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 1 | 0.9 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 1 | 0.9 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 1 | 0.9 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 18 | 0.9 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 18 | 0.9 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 18 | 0.9 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 5 | 0.9 |
| (1,2304) | 1:132:A:SER:HA | 1:136:A:GLN:HG2 | 8 | 0.9 |
| (1,2168) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HG2 | 20 | 0.9 |
| (1,2168) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HG2 | 20 | 0.9 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 14 | 0.9 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 9 | 0.9 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB2 | 9 | 0.9 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB3 | 9 | 0.9 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 2 | 0.9 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 2 | 0.9 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 2 | 0.9 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 20 | 0.9 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 20 | 0.9 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 20 | 0.9 |
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 14 | 0.9 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 18 | 0.9 |
| (1,1577) | 1:152:A:MET:HB3 | 1:160:A:LEU:HB2 | 2 | 0.9 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 16 | 0.9 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 16 | 0.9 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 16 | 0.9 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 15 | 0.9 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 18 | 0.9 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 18 | 0.9 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 18 | 0.9 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 10 | 0.9 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 10 | 0.9 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 10 | 0.9 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG21 | 12 | 0.9 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG22 | 12 | 0.9 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG23 | 12 | 0.9 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG21 | 12 | 0.9 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG22 | 12 | 0.9 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG23 | 12 | 0.9 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 1 | 0.9 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 13 | 0.9 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 13 | 0.9 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 13 | 0.9 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 13 | 0.9 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 13 | 0.9 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 13 | 0.9 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 16 | 0.9 |
| (1,1084) | 1:37:A:GLU:HG3 | 1:38:A:GLU:H | 9 | 0.9 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 1 | 0.9 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 1 | 0.9 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 1 | 0.9 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 11 | 0.9 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 11 | 0.9 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 11 | 0.9 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 13 | 0.9 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 13 | 0.9 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 13 | 0.9 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 16 | 0.9 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 16 | 0.9 |
| (1,112) | 1:105:A:ALA:H | 1:106:A:ASP:HB3 | 14 | 0.9 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 9 | 0.89 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 9 | 0.89 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 6 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 6 | 0.89 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 7 | 0.89 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 7 | 0.89 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 18 | 0.89 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 18 | 0.89 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 18 | 0.89 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 18 | 0.89 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 18 | 0.89 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 18 | 0.89 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 16 | 0.89 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 16 | 0.89 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 16 | 0.89 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 16 | 0.89 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 16 | 0.89 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 16 | 0.89 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 1 | 0.89 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 3 | 0.89 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 3 | 0.89 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 3 | 0.89 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 6 | 0.89 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 6 | 0.89 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 6 | 0.89 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 11 | 0.89 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 11 | 0.89 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 11 | 0.89 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 9 | 0.89 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 9 | 0.89 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 9 | 0.89 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 9 | 0.89 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 9 | 0.89 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 9 | 0.89 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 9 | 0.89 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 9 | 0.89 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 9 | 0.89 |
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 14 | 0.89 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 14 | 0.89 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 14 | 0.89 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 4 | 0.89 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 4 | 0.89 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 4 | 0.89 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 11 | 0.89 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 11 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 11 | 0.89 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 6 | 0.89 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 6 | 0.89 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 6 | 0.89 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 16 | 0.89 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 16 | 0.89 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 16 | 0.89 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 18 | 0.89 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 18 | 0.89 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 18 | 0.89 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 16 | 0.89 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 16 | 0.89 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 16 | 0.89 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 10 | 0.89 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 10 | 0.89 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 10 | 0.89 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 20 | 0.89 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 20 | 0.89 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 20 | 0.89 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 7 | 0.89 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB2 | 8 | 0.89 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB3 | 8 | 0.89 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD1 | 18 | 0.89 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD2 | 18 | 0.89 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 17 | 0.89 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 17 | 0.89 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 17 | 0.89 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 6 | 0.89 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 8 | 0.89 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 8 | 0.89 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 8 | 0.89 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 8 | 0.89 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 8 | 0.89 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 8 | 0.89 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 18 | 0.89 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 6 | 0.89 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 6 | 0.89 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 6 | 0.89 |
| (1,1669) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HG2 | 4 | 0.89 |
| (1,1669) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HG2 | 4 | 0.89 |
| (1,1669) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HG2 | 4 | 0.89 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB2 | 20 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB3 | 20 | 0.89 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 14 | 0.89 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 14 | 0.89 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 14 | 0.89 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 5 | 0.89 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 9 | 0.89 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 10 | 0.89 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 10 | 0.89 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG11 | 13 | 0.89 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG12 | 13 | 0.89 |
| (1,1295) | 1:40:A:LEU:HB2 | 1:42:A:VAL:HG13 | 13 | 0.89 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 17 | 0.89 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 17 | 0.89 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 17 | 0.89 |
| (1,1213) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE21 | 3 | 0.89 |
| (1,1213) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE21 | 3 | 0.89 |
| (1,1213) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE21 | 3 | 0.89 |
| (1,1058) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HA | 3 | 0.89 |
| (1,883) | 1:49:A:LYS:H | 1:49:A:LYS:HD3 | 20 | 0.89 |
| (1,778) | 1:51:A:PRO:HB3 | 1:54:A:THR:H | 9 | 0.89 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 18 | 0.89 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 18 | 0.89 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 18 | 0.89 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 9 | 0.89 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 9 | 0.89 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 9 | 0.89 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 11 | 0.89 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 11 | 0.89 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 11 | 0.89 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 2 | 0.89 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 2 | 0.89 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 2 | 0.89 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 6 | 0.89 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 6 | 0.89 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 6 | 0.89 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 14 | 0.89 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 14 | 0.89 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 14 | 0.89 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 7 | 0.89 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 7 | 0.89 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 7 | 0.89 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 13 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 13 | 0.89 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 13 | 0.89 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 15 | 0.89 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 15 | 0.89 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 15 | 0.89 |
| (1,163) | 1:69:A:LYS:H | 1:70:A:ASP:HB3 | 13 | 0.89 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 1 | 0.89 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 1 | 0.89 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 15 | 0.88 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE1 | 16 | 0.88 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE2 | 16 | 0.88 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 9 | 0.88 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 9 | 0.88 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 9 | 0.88 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 17 | 0.88 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 17 | 0.88 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 17 | 0.88 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 17 | 0.88 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 17 | 0.88 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 17 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 6 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 6 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 6 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 6 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 6 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 6 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 9 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 9 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 9 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 9 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 9 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 9 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 10 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 10 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 10 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 10 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 10 | 0.88 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 10 | 0.88 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 16 | 0.88 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 5 | 0.88 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 5 | 0.88 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 5 | 0.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 9 | 0.88 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 9 | 0.88 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 9 | 0.88 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 15 | 0.88 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 15 | 0.88 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 15 | 0.88 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 15 | 0.88 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 15 | 0.88 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 15 | 0.88 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 15 | 0.88 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 15 | 0.88 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 15 | 0.88 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG11 | 4 | 0.88 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG12 | 4 | 0.88 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG13 | 4 | 0.88 |
| (1,2945) | 1:23:A:LEU:HD21 | 1:58:A:LYS:HA | 5 | 0.88 |
| (1,2945) | 1:23:A:LEU:HD22 | 1:58:A:LYS:HA | 5 | 0.88 |
| (1,2945) | 1:23:A:LEU:HD23 | 1:58:A:LYS:HA | 5 | 0.88 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 17 | 0.88 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 17 | 0.88 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 17 | 0.88 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 19 | 0.88 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 19 | 0.88 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 19 | 0.88 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 19 | 0.88 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 19 | 0.88 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 19 | 0.88 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG11 | 1 | 0.88 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG12 | 1 | 0.88 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG13 | 1 | 0.88 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG11 | 2 | 0.88 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG12 | 2 | 0.88 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG13 | 2 | 0.88 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 15 | 0.88 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 15 | 0.88 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 15 | 0.88 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG11 | 12 | 0.88 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG12 | 12 | 0.88 |
| (1,2045) | 1:27:A:SER:HB3 | 1:61:A:VAL:HG13 | 12 | 0.88 |
| (1,1990) | 1:133:A:LEU:HB3 | 1:136:A:GLN:HB2 | 2 | 0.88 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 6 | 0.88 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 6 | 0.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 6 | 0.88 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 19 | 0.88 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 20 | 0.88 |
| (1,1663) | 1:72:A:THR:HG21 | 1:138:A:GLU:HG3 | 13 | 0.88 |
| (1,1663) | 1:72:A:THR:HG22 | 1:138:A:GLU:HG3 | 13 | 0.88 |
| (1,1663) | 1:72:A:THR:HG23 | 1:138:A:GLU:HG3 | 13 | 0.88 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 12 | 0.88 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 12 | 0.88 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 12 | 0.88 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 17 | 0.88 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 17 | 0.88 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 17 | 0.88 |
| (1,1409) | 1:67:A:LEU:HB2 | 1:70:A:ASP:HB3 | 13 | 0.88 |
| (1,1358) | 1:179:A:ASP:HB3 | 1:183:A:GLN:HE21 | 17 | 0.88 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 3 | 0.88 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 16 | 0.88 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 16 | 0.88 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 16 | 0.88 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD21 | 1 | 0.88 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD22 | 1 | 0.88 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD23 | 1 | 0.88 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 13 | 0.88 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 13 | 0.88 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 13 | 0.88 |
| (1,683) | 1:168:A:SER:H | 1:170:A:MET:HG2 | 9 | 0.88 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 3 | 0.88 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 3 | 0.88 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 3 | 0.88 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 19 | 0.88 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 19 | 0.88 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 19 | 0.88 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 16 | 0.88 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 16 | 0.88 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 16 | 0.88 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 2 | 0.88 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 18 | 0.88 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 18 | 0.88 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 18 | 0.88 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE1 | 15 | 0.87 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE2 | 15 | 0.87 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE1 | 15 | 0.87 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE2 | 15 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE1 | 15 | 0.87 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE2 | 15 | 0.87 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 7 | 0.87 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 7 | 0.87 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 6 | 0.87 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 6 | 0.87 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 1 | 0.87 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 1 | 0.87 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 2 | 0.87 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 2 | 0.87 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 18 | 0.87 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 18 | 0.87 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 1 | 0.87 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 9 | 0.87 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 11 | 0.87 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 11 | 0.87 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 11 | 0.87 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 1 | 0.87 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 1 | 0.87 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 1 | 0.87 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 1 | 0.87 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 1 | 0.87 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 1 | 0.87 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 2 | 0.87 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 2 | 0.87 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 5 | 0.87 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 5 | 0.87 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 5 | 0.87 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 5 | 0.87 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 5 | 0.87 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 5 | 0.87 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 9 | 0.87 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 1 | 0.87 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 1 | 0.87 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 1 | 0.87 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 12 | 0.87 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 12 | 0.87 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 12 | 0.87 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 12 | 0.87 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 12 | 0.87 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 12 | 0.87 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 12 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 12 | 0.87 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 12 | 0.87 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 14 | 0.87 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 14 | 0.87 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 14 | 0.87 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 14 | 0.87 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 14 | 0.87 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 14 | 0.87 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 14 | 0.87 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 14 | 0.87 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 14 | 0.87 |
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 10 | 0.87 |
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 11 | 0.87 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 9 | 0.87 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 9 | 0.87 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 9 | 0.87 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 19 | 0.87 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 19 | 0.87 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 19 | 0.87 |
| (1,2632) | 1:101:A:VAL:HG21 | 1:107:A:ILE:H | 7 | 0.87 |
| (1,2632) | 1:101:A:VAL:HG22 | 1:107:A:ILE:H | 7 | 0.87 |
| (1,2632) | 1:101:A:VAL:HG23 | 1:107:A:ILE:H | 7 | 0.87 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 7 | 0.87 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 7 | 0.87 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 7 | 0.87 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 11 | 0.87 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 11 | 0.87 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 11 | 0.87 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 17 | 0.87 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 17 | 0.87 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 17 | 0.87 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 20 | 0.87 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 20 | 0.87 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 20 | 0.87 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 4 | 0.87 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 4 | 0.87 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 4 | 0.87 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 14 | 0.87 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 14 | 0.87 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 14 | 0.87 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 5 | 0.87 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 14 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 10 | 0.87 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 10 | 0.87 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 10 | 0.87 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 10 | 0.87 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 10 | 0.87 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 10 | 0.87 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 11 | 0.87 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 17 | 0.87 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 10 | 0.87 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 9 | 0.87 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 19 | 0.87 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 8 | 0.87 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 8 | 0.87 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 8 | 0.87 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 4 | 0.87 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 13 | 0.87 |
| (1,1632) | 1:31:A:PRO:HA | 1:96:A:GLN:HG2 | 3 | 0.87 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB2 | 11 | 0.87 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB3 | 11 | 0.87 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 11 | 0.87 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 9 | 0.87 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 9 | 0.87 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 9 | 0.87 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 1 | 0.87 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 1 | 0.87 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 1 | 0.87 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 11 | 0.87 |
| (1,1058) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HA | 15 | 0.87 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 5 | 0.87 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 5 | 0.87 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 5 | 0.87 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 4 | 0.87 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 1 | 0.87 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 1 | 0.87 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 1 | 0.87 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 1 | 0.87 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 3 | 0.87 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 4 | 0.87 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 4 | 0.87 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 4 | 0.87 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 6 | 0.87 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 6 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 6 | 0.87 |
| (1,163) | 1:69:A:LYS:H | 1:70:A:ASP:HB3 | 4 | 0.87 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 6 | 0.86 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 6 | 0.86 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 6 | 0.86 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 6 | 0.86 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 6 | 0.86 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 6 | 0.86 |
| (1,3442) | 1:73:A:GLN:HG2 | 1:125:A:TRP:HH2 | 18 | 0.86 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 15 | 0.86 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 15 | 0.86 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 15 | 0.86 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 15 | 0.86 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 15 | 0.86 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 15 | 0.86 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 12 | 0.86 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE1 | 12 | 0.86 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE2 | 12 | 0.86 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE3 | 12 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 1 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 1 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 1 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 1 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 1 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 1 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 1 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 1 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 1 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 5 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 5 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 5 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 5 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 5 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 5 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 5 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 5 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 5 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 16 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 16 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 16 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 16 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 16 | 0.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 16 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 16 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 16 | 0.86 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 16 | 0.86 |
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 5 | 0.86 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 5 | 0.86 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 5 | 0.86 |
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 16 | 0.86 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 16 | 0.86 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 1 | 0.86 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 1 | 0.86 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 1 | 0.86 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 1 | 0.86 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 1 | 0.86 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 1 | 0.86 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 1 | 0.86 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 1 | 0.86 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 1 | 0.86 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 18 | 0.86 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 18 | 0.86 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 18 | 0.86 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 1 | 0.86 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 1 | 0.86 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 1 | 0.86 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 6 | 0.86 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 6 | 0.86 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 6 | 0.86 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 14 | 0.86 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 14 | 0.86 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 14 | 0.86 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 14 | 0.86 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 14 | 0.86 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 14 | 0.86 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 2 | 0.86 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 2 | 0.86 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 2 | 0.86 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 14 | 0.86 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 14 | 0.86 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 14 | 0.86 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 14 | 0.86 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 14 | 0.86 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 14 | 0.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 12 | 0.86 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 12 | 0.86 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 12 | 0.86 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 6 | 0.86 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 6 | 0.86 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 6 | 0.86 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 9 | 0.86 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 9 | 0.86 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 9 | 0.86 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 20 | 0.86 |
| (1,2345) | 1:7:A:LYS:HG3 | 1:8:A:GLN:HB2 | 10 | 0.86 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 12 | 0.86 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 12 | 0.86 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 12 | 0.86 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 17 | 0.86 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 7 | 0.86 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 17 | 0.86 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 7 | 0.86 |
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 4 | 0.86 |
| (1,1785) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD2 | 18 | 0.86 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 9 | 0.86 |
| (1,1669) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HG2 | 6 | 0.86 |
| (1,1669) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HG2 | 6 | 0.86 |
| (1,1669) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HG2 | 6 | 0.86 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 17 | 0.86 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 17 | 0.86 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 17 | 0.86 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 6 | 0.86 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 4 | 0.86 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 4 | 0.86 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 4 | 0.86 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 9 | 0.86 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 9 | 0.86 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 9 | 0.86 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 12 | 0.86 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 12 | 0.86 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 12 | 0.86 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 9 | 0.86 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 13 | 0.86 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 15 | 0.86 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 15 | 0.86 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 15 | 0.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,991) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HD22 | 1 | 0.86 |
| (1,894) | 1:103:A:SER:H | 1:106:A:ASP:HB3 | 5 | 0.86 |
| (1,883) | 1:49:A:LYS:H | 1:49:A:LYS:HD3 | 12 | 0.86 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 18 | 0.86 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 18 | 0.86 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 18 | 0.86 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 20 | 0.86 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 3 | 0.86 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 3 | 0.86 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 3 | 0.86 |
| (1,683) | 1:168:A:SER:H | 1:170:A:MET:HG2 | 14 | 0.86 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 9 | 0.86 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 9 | 0.86 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 9 | 0.86 |
| (1,416) | 1:122:A:ASP:HB3 | 1:123:A:ALA:H | 7 | 0.86 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 8 | 0.86 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 8 | 0.86 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 8 | 0.86 |
| (1,163) | 1:69:A:LYS:H | 1:70:A:ASP:HB3 | 12 | 0.86 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 9 | 0.86 |
| (1,128) | 1:12:A:LEU:HD11 | 1:159:A:GLN:H | 14 | 0.86 |
| (1,128) | 1:12:A:LEU:HD12 | 1:159:A:GLN:H | 14 | 0.86 |
| (1,128) | 1:12:A:LEU:HD13 | 1:159:A:GLN:H | 14 | 0.86 |
| (1,112) | 1:105:A:ALA:H | 1:106:A:ASP:HB3 | 11 | 0.86 |
| (1,90) | 1:185:A:VAL:HA | 1:188:A:LYS:H | 6 | 0.86 |
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 14 | 0.85 |
| (1,3495) | 1:23:A:LEU:HD21 | 1:59:A:TYR:HE1 | 10 | 0.85 |
| (1,3495) | 1:23:A:LEU:HD21 | 1:59:A:TYR:HE2 | 10 | 0.85 |
| (1,3495) | 1:23:A:LEU:HD22 | 1:59:A:TYR:HE1 | 10 | 0.85 |
| (1,3495) | 1:23:A:LEU:HD22 | 1:59:A:TYR:HE2 | 10 | 0.85 |
| (1,3495) | 1:23:A:LEU:HD23 | 1:59:A:TYR:HE1 | 10 | 0.85 |
| (1,3495) | 1:23:A:LEU:HD23 | 1:59:A:TYR:HE2 | 10 | 0.85 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 2 | 0.85 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 9 | 0.85 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE1 | 12 | 0.85 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE2 | 12 | 0.85 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 4 | 0.85 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 4 | 0.85 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 4 | 0.85 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 4 | 0.85 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 4 | 0.85 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 4 | 0.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 4 | 0.85 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 4 | 0.85 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 6 | 0.85 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 13 | 0.85 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 18 | 0.85 |
| (1,3267) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HD11 | 18 | 0.85 |
| (1,3267) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HD12 | 18 | 0.85 |
| (1,3267) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HD13 | 18 | 0.85 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 13 | 0.85 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 13 | 0.85 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 13 | 0.85 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 13 | 0.85 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 13 | 0.85 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 13 | 0.85 |
| (1,3076) | 1:47:A:ARG:HG3 | 1:56:A:MET:HE1 | 10 | 0.85 |
| (1,3076) | 1:47:A:ARG:HG3 | 1:56:A:MET:HE2 | 10 | 0.85 |
| (1,3076) | 1:47:A:ARG:HG3 | 1:56:A:MET:HE3 | 10 | 0.85 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE1 | 7 | 0.85 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE2 | 7 | 0.85 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE3 | 7 | 0.85 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 10 | 0.85 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 10 | 0.85 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 10 | 0.85 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 10 | 0.85 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 10 | 0.85 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 10 | 0.85 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 10 | 0.85 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 10 | 0.85 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 10 | 0.85 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG11 | 8 | 0.85 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG12 | 8 | 0.85 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG13 | 8 | 0.85 |
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 19 | 0.85 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 5 | 0.85 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 19 | 0.85 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 19 | 0.85 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 19 | 0.85 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 11 | 0.85 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 11 | 0.85 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 11 | 0.85 |
| (1,2621) | 1:101:A:VAL:HG21 | 1:106:A:ASP:H | 7 | 0.85 |
| (1,2621) | 1:101:A:VAL:HG22 | 1:106:A:ASP:H | 7 | 0.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2621) | 1:101:A:VAL:HG23 | 1:106:A:ASP:H | 7 | 0.85 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 10 | 0.85 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 10 | 0.85 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 10 | 0.85 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG21 | 4 | 0.85 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG22 | 4 | 0.85 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG23 | 4 | 0.85 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 5 | 0.85 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 5 | 0.85 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 5 | 0.85 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 18 | 0.85 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 18 | 0.85 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 18 | 0.85 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 10 | 0.85 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 10 | 0.85 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 10 | 0.85 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 10 | 0.85 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 10 | 0.85 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 10 | 0.85 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 10 | 0.85 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 1 | 0.85 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 1 | 0.85 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 1 | 0.85 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 1 | 0.85 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 1 | 0.85 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 1 | 0.85 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 20 | 0.85 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD1 | 8 | 0.85 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD2 | 8 | 0.85 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 10 | 0.85 |
| (1,1963) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HD2 | 17 | 0.85 |
| (1,1963) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HD3 | 17 | 0.85 |
| (1,1890) | 1:36:A:PHE:H | 1:37:A:GLU:HB2 | 13 | 0.85 |
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 3 | 0.85 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 12 | 0.85 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 12 | 0.85 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 12 | 0.85 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD1 | 16 | 0.85 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD2 | 16 | 0.85 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE1 | 9 | 0.85 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE2 | 9 | 0.85 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 13 | 0.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 10 | 0.85 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 10 | 0.85 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 10 | 0.85 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 8 | 0.85 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 8 | 0.85 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 8 | 0.85 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 17 | 0.85 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 11 | 0.85 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 11 | 0.85 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 11 | 0.85 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 11 | 0.85 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 11 | 0.85 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 11 | 0.85 |
| (1,1084) | 1:37:A:GLU:HG3 | 1:38:A:GLU:H | 7 | 0.85 |
| (1,1058) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HA | 7 | 0.85 |
| (1,1058) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HA | 16 | 0.85 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 17 | 0.85 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 17 | 0.85 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 17 | 0.85 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 14 | 0.85 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 14 | 0.85 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 14 | 0.85 |
| (1,894) | 1:103:A:SER:H | 1:106:A:ASP:HB3 | 19 | 0.85 |
| (1,778) | 1:51:A:PRO:HB3 | 1:54:A:THR:H | 7 | 0.85 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 20 | 0.85 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 20 | 0.85 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 20 | 0.85 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 5 | 0.85 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 5 | 0.85 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 5 | 0.85 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 20 | 0.85 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 20 | 0.85 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 20 | 0.85 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 1 | 0.85 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 1 | 0.85 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 1 | 0.85 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 7 | 0.85 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 7 | 0.85 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 15 | 0.84 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 15 | 0.84 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 15 | 0.84 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 15 | 0.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 17 | 0.84 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 7 | 0.84 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 17 | 0.84 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 3 | 0.84 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 3 | 0.84 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 9 | 0.84 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 1 | 0.84 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 1 | 0.84 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 1 | 0.84 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 1 | 0.84 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 1 | 0.84 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 1 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 8 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 8 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 8 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 8 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 8 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 8 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 8 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 8 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 8 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 17 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 17 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 17 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 17 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 17 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 17 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 17 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 17 | 0.84 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 17 | 0.84 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 14 | 0.84 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 19 | 0.84 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 14 | 0.84 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 14 | 0.84 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 14 | 0.84 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 18 | 0.84 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 18 | 0.84 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 18 | 0.84 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 12 | 0.84 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 12 | 0.84 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 12 | 0.84 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 5 | 0.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 8 | 0.84 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 8 | 0.84 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 8 | 0.84 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 1 | 0.84 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 1 | 0.84 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 1 | 0.84 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 17 | 0.84 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 17 | 0.84 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 17 | 0.84 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 11 | 0.84 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 11 | 0.84 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 11 | 0.84 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 3 | 0.84 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 3 | 0.84 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 3 | 0.84 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 15 | 0.84 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 12 | 0.84 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 19 | 0.84 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 19 | 0.84 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 19 | 0.84 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 18 | 0.84 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 1 | 0.84 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 8 | 0.84 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 20 | 0.84 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 6 | 0.84 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 6 | 0.84 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 6 | 0.84 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG12 | 13 | 0.84 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG13 | 13 | 0.84 |
| (1,1669) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HG2 | 11 | 0.84 |
| (1,1669) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HG2 | 11 | 0.84 |
| (1,1669) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HG2 | 11 | 0.84 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 6 | 0.84 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 6 | 0.84 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 6 | 0.84 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 20 | 0.84 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 20 | 0.84 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 3 | 0.84 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 3 | 0.84 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 3 | 0.84 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 6 | 0.84 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 8 | 0.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 8 | 0.84 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 8 | 0.84 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 12 | 0.84 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 12 | 0.84 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 12 | 0.84 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 19 | 0.84 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 19 | 0.84 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 19 | 0.84 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 2 | 0.84 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 2 | 0.84 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 2 | 0.84 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 3 | 0.84 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 5 | 0.84 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 6 | 0.84 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 9 | 0.84 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 10 | 0.84 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 12 | 0.84 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 13 | 0.84 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 15 | 0.84 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 14 | 0.84 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 14 | 0.84 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 14 | 0.84 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 11 | 0.84 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 10 | 0.83 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 10 | 0.83 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 11 | 0.83 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 11 | 0.83 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 19 | 0.83 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 19 | 0.83 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 14 | 0.83 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 14 | 0.83 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 14 | 0.83 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE1 | 2 | 0.83 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE2 | 2 | 0.83 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE3 | 2 | 0.83 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG11 | 11 | 0.83 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG12 | 11 | 0.83 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG13 | 11 | 0.83 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 5 | 0.83 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 5 | 0.83 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 5 | 0.83 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 5 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 5 | 0.83 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 5 | 0.83 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 5 | 0.83 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 5 | 0.83 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 5 | 0.83 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 1 | 0.83 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 8 | 0.83 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 8 | 0.83 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 8 | 0.83 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 7 | 0.83 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 7 | 0.83 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 7 | 0.83 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 2 | 0.83 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 2 | 0.83 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 2 | 0.83 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 18 | 0.83 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 18 | 0.83 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 18 | 0.83 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 15 | 0.83 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 15 | 0.83 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 15 | 0.83 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 2 | 0.83 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 2 | 0.83 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 2 | 0.83 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 1 | 0.83 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 1 | 0.83 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 1 | 0.83 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 15 | 0.83 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 15 | 0.83 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 15 | 0.83 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 2 | 0.83 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 2 | 0.83 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 2 | 0.83 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 5 | 0.83 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 5 | 0.83 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 5 | 0.83 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 5 | 0.83 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 5 | 0.83 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 5 | 0.83 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 16 | 0.83 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 16 | 0.83 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 16 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 13 | 0.83 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 13 | 0.83 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 13 | 0.83 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 11 | 0.83 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 11 | 0.83 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 11 | 0.83 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 20 | 0.83 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 20 | 0.83 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 20 | 0.83 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 20 | 0.83 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 20 | 0.83 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 20 | 0.83 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 2 | 0.83 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 5 | 0.83 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 12 | 0.83 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 3 | 0.83 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 3 | 0.83 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 3 | 0.83 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG12 | 14 | 0.83 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG13 | 14 | 0.83 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 19 | 0.83 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 12 | 0.83 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 12 | 0.83 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 12 | 0.83 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 20 | 0.83 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 20 | 0.83 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 20 | 0.83 |
| (1,1366) | 1:34:A:TYR:HE1 | 1:97:A:LYS:HE3 | 16 | 0.83 |
| (1,1366) | 1:34:A:TYR:HE2 | 1:97:A:LYS:HE3 | 16 | 0.83 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 6 | 0.83 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 6 | 0.83 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 6 | 0.83 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 12 | 0.83 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 12 | 0.83 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 12 | 0.83 |
| (1,883) | 1:49:A:LYS:H | 1:49:A:LYS:HD3 | 7 | 0.83 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 17 | 0.83 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 7 | 0.83 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 7 | 0.83 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 7 | 0.83 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 14 | 0.83 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 14 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 14 | 0.83 |
| (1,683) | 1:168:A:SER:H | 1:170:A:MET:HG2 | 17 | 0.83 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 8 | 0.83 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 18 | 0.83 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 20 | 0.83 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 13 | 0.83 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 18 | 0.83 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 18 | 0.83 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 18 | 0.83 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 14 | 0.83 |
| (1,102) | 1:50:A:LEU:HD21 | 1:56:A:MET:H | 2 | 0.83 |
| (1,102) | 1:50:A:LEU:HD22 | 1:56:A:MET:H | 2 | 0.83 |
| (1,102) | 1:50:A:LEU:HD23 | 1:56:A:MET:H | 2 | 0.83 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 2 | 0.82 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 2 | 0.82 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 2 | 0.82 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 2 | 0.82 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 2 | 0.82 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 2 | 0.82 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 14 | 0.82 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 1 | 0.82 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 1 | 0.82 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 1 | 0.82 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 1 | 0.82 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 1 | 0.82 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 1 | 0.82 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 3 | 0.82 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 18 | 0.82 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 18 | 0.82 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 18 | 0.82 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 18 | 0.82 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 18 | 0.82 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 18 | 0.82 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 18 | 0.82 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 18 | 0.82 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 18 | 0.82 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 18 | 0.82 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 18 | 0.82 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 18 | 0.82 |
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 15 | 0.82 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 15 | 0.82 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 15 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 19 | 0.82 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 19 | 0.82 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 19 | 0.82 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 11 | 0.82 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 11 | 0.82 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 11 | 0.82 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 6 | 0.82 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 9 | 0.82 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 11 | 0.82 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 10 | 0.82 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 10 | 0.82 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 10 | 0.82 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG11 | 7 | 0.82 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG12 | 7 | 0.82 |
| (1,2729) | 1:38:A:GLU:H | 1:39:A:VAL:HG13 | 7 | 0.82 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 1 | 0.82 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 1 | 0.82 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 1 | 0.82 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 4 | 0.82 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 4 | 0.82 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 4 | 0.82 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 3 | 0.82 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 3 | 0.82 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 3 | 0.82 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 6 | 0.82 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 6 | 0.82 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 6 | 0.82 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD21 | 17 | 0.82 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD22 | 17 | 0.82 |
| (1,2488) | 1:8:A:GLN:HA | 1:160:A:LEU:HD23 | 17 | 0.82 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 5 | 0.82 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 5 | 0.82 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 5 | 0.82 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 16 | 0.82 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 16 | 0.82 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 16 | 0.82 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 5 | 0.82 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 2 | 0.82 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 9 | 0.82 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 18 | 0.82 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 18 | 0.82 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 18 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2291) | 1:117:A:LYS:HG3 | 1:120:A:ASP:H | 12 | 0.82 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 9 | 0.82 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 9 | 0.82 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 9 | 0.82 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 9 | 0.82 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 9 | 0.82 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 9 | 0.82 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 3 | 0.82 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 13 | 0.82 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 13 | 0.82 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 8 | 0.82 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 8 | 0.82 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 8 | 0.82 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 3 | 0.82 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 3 | 0.82 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 3 | 0.82 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG21 | 9 | 0.82 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG22 | 9 | 0.82 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG23 | 9 | 0.82 |
| (1,1833) | 1:116:A:VAL:HA | 1:117:A:LYS:HB3 | 5 | 0.82 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 1 | 0.82 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 1 | 0.82 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 1 | 0.82 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE1 | 19 | 0.82 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE2 | 19 | 0.82 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB2 | 14 | 0.82 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB3 | 14 | 0.82 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 14 | 0.82 |
| (1,1577) | 1:152:A:MET:HB3 | 1:160:A:LEU:HB2 | 15 | 0.82 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 4 | 0.82 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 13 | 0.82 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 13 | 0.82 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 13 | 0.82 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 15 | 0.82 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 15 | 0.82 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 15 | 0.82 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 7 | 0.82 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 13 | 0.82 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 13 | 0.82 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 13 | 0.82 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 4 | 0.82 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 4 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 4 | 0.82 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 10 | 0.82 |
| (1,1080) | 1:34:A:TYR:HD2 | 1:38:A:GLU:H | 3 | 0.82 |
| (1,683) | 1:168:A:SER:H | 1:170:A:MET:HG2 | 11 | 0.82 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 2 | 0.82 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 4 | 0.82 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 17 | 0.82 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 8 | 0.82 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 5 | 0.82 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 5 | 0.82 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 5 | 0.82 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 7 | 0.82 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 7 | 0.82 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 7 | 0.82 |
| (1,102) | 1:50:A:LEU:HD21 | 1:56:A:MET:H | 10 | 0.82 |
| (1,102) | 1:50:A:LEU:HD22 | 1:56:A:MET:H | 10 | 0.82 |
| (1,102) | 1:50:A:LEU:HD23 | 1:56:A:MET:H | 10 | 0.82 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 3 | 0.81 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 3 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 1 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 1 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 1 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 1 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 1 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 1 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 9 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 9 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 9 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 9 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 9 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 9 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 13 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 13 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 13 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 13 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 13 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 13 | 0.81 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 13 | 0.81 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 13 | 0.81 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 1 | 0.81 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 12 | 0.81 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 12 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 12 | 0.81 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 11 | 0.81 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 14 | 0.81 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 19 | 0.81 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 19 | 0.81 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 19 | 0.81 |
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 4 | 0.81 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 15 | 0.81 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 13 | 0.81 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 13 | 0.81 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 13 | 0.81 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 13 | 0.81 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 13 | 0.81 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 13 | 0.81 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 6 | 0.81 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 6 | 0.81 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 6 | 0.81 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 4 | 0.81 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 4 | 0.81 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 4 | 0.81 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 16 | 0.81 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 16 | 0.81 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 16 | 0.81 |
| (1,2629) | 1:101:A:VAL:HG21 | 1:102:A:GLN:HA | 20 | 0.81 |
| (1,2629) | 1:101:A:VAL:HG22 | 1:102:A:GLN:HA | 20 | 0.81 |
| (1,2629) | 1:101:A:VAL:HG23 | 1:102:A:GLN:HA | 20 | 0.81 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 16 | 0.81 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 16 | 0.81 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 16 | 0.81 |
| (1,2538) | 1:23:A:LEU:HD11 | 1:153:A:TYR:H | 6 | 0.81 |
| (1,2538) | 1:23:A:LEU:HD12 | 1:153:A:TYR:H | 6 | 0.81 |
| (1,2538) | 1:23:A:LEU:HD13 | 1:153:A:TYR:H | 6 | 0.81 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 18 | 0.81 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 18 | 0.81 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 18 | 0.81 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 20 | 0.81 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 8 | 0.81 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 8 | 0.81 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 8 | 0.81 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 2 | 0.81 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 13 | 0.81 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 6 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 20 | 0.81 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 20 | 0.81 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 20 | 0.81 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 20 | 0.81 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 20 | 0.81 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 20 | 0.81 |
| (1,1899) | 1:146:A:LEU:HA | 1:147:A:GLN:HB3 | 14 | 0.81 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 1 | 0.81 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 16 | 0.81 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 18 | 0.81 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 11 | 0.81 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 11 | 0.81 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 11 | 0.81 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 11 | 0.81 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 11 | 0.81 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 11 | 0.81 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 8 | 0.81 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 9 | 0.81 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 18 | 0.81 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 12 | 0.81 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 12 | 0.81 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 12 | 0.81 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG11 | 9 | 0.81 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG12 | 9 | 0.81 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG13 | 9 | 0.81 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 6 | 0.81 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 6 | 0.81 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 6 | 0.81 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 2 | 0.81 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 2 | 0.81 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 2 | 0.81 |
| (1,894) | 1:103:A:SER:H | 1:106:A:ASP:HB3 | 18 | 0.81 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 1 | 0.81 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 14 | 0.81 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 16 | 0.81 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 20 | 0.81 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 20 | 0.81 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 20 | 0.81 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 11 | 0.81 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 12 | 0.81 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 10 | 0.81 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 15 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 16 | 0.81 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 11 | 0.81 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 11 | 0.81 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 11 | 0.81 |
| (1,128) | 1:12:A:LEU:HD11 | 1:159:A:GLN:H | 7 | 0.81 |
| (1,128) | 1:12:A:LEU:HD12 | 1:159:A:GLN:H | 7 | 0.81 |
| (1,128) | 1:12:A:LEU:HD13 | 1:159:A:GLN:H | 7 | 0.81 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG11 | 10 | 0.81 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG12 | 10 | 0.81 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG13 | 10 | 0.81 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 1 | 0.81 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 4 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 4 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 4 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 4 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 4 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 4 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 10 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 10 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 10 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 10 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 10 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 10 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 12 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 12 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 12 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 12 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 12 | 0.8 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 12 | 0.8 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 2 | 0.8 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 2 | 0.8 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 4 | 0.8 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 4 | 0.8 |
| (1,3415) | 1:59:A:TYR:HD1 | 1:137:A:GLN:HG3 | 13 | 0.8 |
| (1,3415) | 1:59:A:TYR:HD2 | 1:137:A:GLN:HG3 | 13 | 0.8 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE1 | 8 | 0.8 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE2 | 8 | 0.8 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 12 | 0.8 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 12 | 0.8 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 2 | 0.8 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 3 | 0.8 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 12 | 0.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 1 | 0.8 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 13 | 0.8 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 12 | 0.8 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 12 | 0.8 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 12 | 0.8 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 13 | 0.8 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 13 | 0.8 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 13 | 0.8 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 5 | 0.8 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 5 | 0.8 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 5 | 0.8 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 5 | 0.8 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 5 | 0.8 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 5 | 0.8 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 5 | 0.8 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 5 | 0.8 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 5 | 0.8 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 4 | 0.8 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 4 | 0.8 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 4 | 0.8 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 12 | 0.8 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 12 | 0.8 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 12 | 0.8 |
| (1,2392) | 1:31:A:PRO:HA | 1:34:A:TYR:HA | 3 | 0.8 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 7 | 0.8 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 13 | 0.8 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 13 | 0.8 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 13 | 0.8 |
| (1,2304) | 1:132:A:SER:HA | 1:136:A:GLN:HG2 | 3 | 0.8 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 8 | 0.8 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 8 | 0.8 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 8 | 0.8 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 8 | 0.8 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 8 | 0.8 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 8 | 0.8 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 10 | 0.8 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 10 | 0.8 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 10 | 0.8 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 20 | 0.8 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB2 | 11 | 0.8 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB3 | 11 | 0.8 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB2 | 11 | 0.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB3 | 11 | 0.8 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB2 | 11 | 0.8 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB3 | 11 | 0.8 |
| (1,1813) | 1:160:A:LEU:HD21 | 1:180:A:THR:HB | 8 | 0.8 |
| (1,1813) | 1:160:A:LEU:HD22 | 1:180:A:THR:HB | 8 | 0.8 |
| (1,1813) | 1:160:A:LEU:HD23 | 1:180:A:THR:HB | 8 | 0.8 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG12 | 15 | 0.8 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG13 | 15 | 0.8 |
| (1,1632) | 1:31:A:PRO:HA | 1:96:A:GLN:HG2 | 13 | 0.8 |
| (1,1577) | 1:152:A:MET:HB3 | 1:160:A:LEU:HB2 | 18 | 0.8 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 3 | 0.8 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 13 | 0.8 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 17 | 0.8 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 17 | 0.8 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 17 | 0.8 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG11 | 13 | 0.8 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG12 | 13 | 0.8 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG13 | 13 | 0.8 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 17 | 0.8 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 17 | 0.8 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 17 | 0.8 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 11 | 0.8 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 11 | 0.8 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 11 | 0.8 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 18 | 0.8 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 5 | 0.8 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 5 | 0.8 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 5 | 0.8 |
| (1,1089) | 1:7:A:LYS:HB2 | 1:9:A:TYR:H | 10 | 0.8 |
| (1,991) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HD22 | 15 | 0.8 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 16 | 0.8 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 16 | 0.8 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 16 | 0.8 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD21 | 6 | 0.8 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD22 | 6 | 0.8 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD23 | 6 | 0.8 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 13 | 0.8 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 16 | 0.8 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 16 | 0.8 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 16 | 0.8 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 11 | 0.8 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 9 | 0.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 6 | 0.8 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 11 | 0.8 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 11 | 0.8 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 11 | 0.8 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 20 | 0.8 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 20 | 0.8 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 20 | 0.8 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 8 | 0.8 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 8 | 0.8 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 8 | 0.8 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 2 | 0.8 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 2 | 0.8 |
| (1,102) | 1:50:A:LEU:HD21 | 1:56:A:MET:H | 1 | 0.8 |
| (1,102) | 1:50:A:LEU:HD22 | 1:56:A:MET:H | 1 | 0.8 |
| (1,102) | 1:50:A:LEU:HD23 | 1:56:A:MET:H | 1 | 0.8 |
| (1,102) | 1:50:A:LEU:HD21 | 1:56:A:MET:H | 13 | 0.8 |
| (1,102) | 1:50:A:LEU:HD22 | 1:56:A:MET:H | 13 | 0.8 |
| (1,102) | 1:50:A:LEU:HD23 | 1:56:A:MET:H | 13 | 0.8 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 7 | 0.79 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 7 | 0.79 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 7 | 0.79 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 7 | 0.79 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 7 | 0.79 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 7 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 6 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 6 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 6 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 6 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 6 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 6 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 11 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 11 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 11 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 11 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 11 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 11 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 18 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 18 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 18 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 18 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 18 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 18 | 0.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB2 | 3 | 0.79 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB3 | 3 | 0.79 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB2 | 3 | 0.79 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB3 | 3 | 0.79 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 1 | 0.79 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 1 | 0.79 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 1 | 0.79 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 1 | 0.79 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 1 | 0.79 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 1 | 0.79 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 16 | 0.79 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 16 | 0.79 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 16 | 0.79 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 16 | 0.79 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 16 | 0.79 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 16 | 0.79 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 4 | 0.79 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 6 | 0.79 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 3 | 0.79 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 3 | 0.79 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 3 | 0.79 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 3 | 0.79 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 3 | 0.79 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 3 | 0.79 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 4 | 0.79 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 5 | 0.79 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 10 | 0.79 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 7 | 0.79 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 7 | 0.79 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 7 | 0.79 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG21 | 11 | 0.79 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG22 | 11 | 0.79 |
| (1,3228) | 1:90:A:PRO:HD3 | 1:110:A:VAL:HG23 | 11 | 0.79 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE1 | 1 | 0.79 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE2 | 1 | 0.79 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE3 | 1 | 0.79 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 7 | 0.79 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 7 | 0.79 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 7 | 0.79 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 7 | 0.79 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 7 | 0.79 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 7 | 0.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 6 | 0.79 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 13 | 0.79 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 13 | 0.79 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 13 | 0.79 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 10 | 0.79 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 10 | 0.79 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 10 | 0.79 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 10 | 0.79 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD11 | 16 | 0.79 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD12 | 16 | 0.79 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD13 | 16 | 0.79 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 5 | 0.79 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 5 | 0.79 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 5 | 0.79 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 2 | 0.79 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 2 | 0.79 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 2 | 0.79 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 16 | 0.79 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 16 | 0.79 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 16 | 0.79 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 8 | 0.79 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 8 | 0.79 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 8 | 0.79 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 8 | 0.79 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 8 | 0.79 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 8 | 0.79 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 8 | 0.79 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 8 | 0.79 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 8 | 0.79 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 14 | 0.79 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 14 | 0.79 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 14 | 0.79 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 20 | 0.79 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 20 | 0.79 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 20 | 0.79 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 17 | 0.79 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 17 | 0.79 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 17 | 0.79 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 4 | 0.79 |
| (1,2308) | 1:131:A:LYS:HG3 | 1:132:A:SER:HA | 19 | 0.79 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 4 | 0.79 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 4 | 0.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 4 | 0.79 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 4 | 0.79 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 4 | 0.79 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 4 | 0.79 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 10 | 0.79 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 10 | 0.79 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 10 | 0.79 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 7 | 0.79 |
| (1,2017) | 1:117:A:LYS:HD3 | 1:120:A:ASP:H | 5 | 0.79 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 11 | 0.79 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 18 | 0.79 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 18 | 0.79 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 18 | 0.79 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 18 | 0.79 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 18 | 0.79 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 18 | 0.79 |
| (1,1813) | 1:160:A:LEU:HD21 | 1:180:A:THR:HB | 18 | 0.79 |
| (1,1813) | 1:160:A:LEU:HD22 | 1:180:A:THR:HB | 18 | 0.79 |
| (1,1813) | 1:160:A:LEU:HD23 | 1:180:A:THR:HB | 18 | 0.79 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 12 | 0.79 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 11 | 0.79 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 11 | 0.79 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 11 | 0.79 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE1 | 7 | 0.79 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE2 | 7 | 0.79 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE1 | 17 | 0.79 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE2 | 17 | 0.79 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 11 | 0.79 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 8 | 0.79 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 8 | 0.79 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 8 | 0.79 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 9 | 0.79 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 9 | 0.79 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 9 | 0.79 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 17 | 0.79 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 17 | 0.79 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 17 | 0.79 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 16 | 0.79 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 11 | 0.79 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 11 | 0.79 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 11 | 0.79 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG11 | 10 | 0.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG12 | 10 | 0.79 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG13 | 10 | 0.79 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 13 | 0.79 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 19 | 0.79 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 9 | 0.79 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 9 | 0.79 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 9 | 0.79 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 16 | 0.79 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 16 | 0.79 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 16 | 0.79 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 2 | 0.79 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 10 | 0.79 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 10 | 0.79 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 10 | 0.79 |
| (1,441) | 1:34:A:TYR:HE1 | 1:92:A:PHE:H | 3 | 0.79 |
| (1,416) | 1:122:A:ASP:HB3 | 1:123:A:ALA:H | 3 | 0.79 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 19 | 0.79 |
| (1,163) | 1:69:A:LYS:H | 1:70:A:ASP:HB3 | 9 | 0.79 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 3 | 0.79 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 3 | 0.79 |
| (1,102) | 1:50:A:LEU:HD21 | 1:56:A:MET:H | 6 | 0.79 |
| (1,102) | 1:50:A:LEU:HD22 | 1:56:A:MET:H | 6 | 0.79 |
| (1,102) | 1:50:A:LEU:HD23 | 1:56:A:MET:H | 6 | 0.79 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG11 | 19 | 0.79 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG12 | 19 | 0.79 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG13 | 19 | 0.79 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 4 | 0.79 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 3 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 3 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 3 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 3 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 3 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 3 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 5 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 5 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 5 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 5 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 5 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 5 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 17 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 17 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 17 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 17 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 17 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 17 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 19 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 19 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 19 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 19 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 19 | 0.78 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 19 | 0.78 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 20 | 0.78 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 20 | 0.78 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 20 | 0.78 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 20 | 0.78 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 20 | 0.78 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 20 | 0.78 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 13 | 0.78 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 13 | 0.78 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 4 | 0.78 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 3 | 0.78 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 11 | 0.78 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 14 | 0.78 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 14 | 0.78 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 10 | 0.78 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 2 | 0.78 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 7 | 0.78 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 7 | 0.78 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 7 | 0.78 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 7 | 0.78 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 7 | 0.78 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 7 | 0.78 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 7 | 0.78 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 7 | 0.78 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 7 | 0.78 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE1 | 15 | 0.78 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE2 | 15 | 0.78 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE3 | 15 | 0.78 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 11 | 0.78 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 11 | 0.78 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 11 | 0.78 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 11 | 0.78 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 11 | 0.78 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 11 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 9 | 0.78 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 9 | 0.78 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 9 | 0.78 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 15 | 0.78 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 15 | 0.78 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 15 | 0.78 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 7 | 0.78 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 7 | 0.78 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 7 | 0.78 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 20 | 0.78 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 20 | 0.78 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 20 | 0.78 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 9 | 0.78 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 9 | 0.78 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 9 | 0.78 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG21 | 12 | 0.78 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG22 | 12 | 0.78 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG23 | 12 | 0.78 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG21 | 12 | 0.78 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG22 | 12 | 0.78 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG23 | 12 | 0.78 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 1 | 0.78 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 1 | 0.78 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 1 | 0.78 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 11 | 0.78 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 11 | 0.78 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 11 | 0.78 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 19 | 0.78 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 19 | 0.78 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 19 | 0.78 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 19 | 0.78 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 19 | 0.78 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 19 | 0.78 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 1 | 0.78 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 1 | 0.78 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 1 | 0.78 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 4 | 0.78 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 4 | 0.78 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 4 | 0.78 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 11 | 0.78 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 7 | 0.78 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 7 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 7 | 0.78 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 7 | 0.78 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 7 | 0.78 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 7 | 0.78 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 12 | 0.78 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 12 | 0.78 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 12 | 0.78 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 12 | 0.78 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 12 | 0.78 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 12 | 0.78 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 3 | 0.78 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 8 | 0.78 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 1 | 0.78 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 1 | 0.78 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 1 | 0.78 |
| (1,1866) | 1:34:A:TYR:HA | 1:37:A:GLU:HB2 | 13 | 0.78 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 17 | 0.78 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 5 | 0.78 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 5 | 0.78 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 3 | 0.78 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 19 | 0.78 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 19 | 0.78 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 15 | 0.78 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 15 | 0.78 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 15 | 0.78 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 11 | 0.78 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 11 | 0.78 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 11 | 0.78 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 6 | 0.78 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 8 | 0.78 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 1 | 0.78 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 5 | 0.78 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 4 | 0.78 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 15 | 0.78 |
| (1,1262) | 1:29:A:TYR:HB3 | 1:64:A:LEU:HB2 | 12 | 0.78 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 9 | 0.78 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 9 | 0.78 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 9 | 0.78 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 7 | 0.78 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 7 | 0.78 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 7 | 0.78 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 8 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 8 | 0.78 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 8 | 0.78 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 10 | 0.78 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 10 | 0.78 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 10 | 0.78 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 7 | 0.78 |
| (1,163) | 1:69:A:LYS:H | 1:70:A:ASP:HB3 | 19 | 0.78 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD21 | 7 | 0.78 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD22 | 7 | 0.78 |
| (1,6) | 1:160:A:LEU:H | 1:184:A:LEU:HD23 | 7 | 0.78 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 5 | 0.77 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 5 | 0.77 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 7 | 0.77 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 7 | 0.77 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 7 | 0.77 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 7 | 0.77 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 20 | 0.77 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 20 | 0.77 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 20 | 0.77 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 20 | 0.77 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 20 | 0.77 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 20 | 0.77 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 4 | 0.77 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 4 | 0.77 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 4 | 0.77 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 4 | 0.77 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 4 | 0.77 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 4 | 0.77 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 20 | 0.77 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 1 | 0.77 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 4 | 0.77 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 8 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 13 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 13 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 13 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 13 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 13 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 13 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 13 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 13 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 13 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 18 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 18 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 18 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 18 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 18 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 18 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 18 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 18 | 0.77 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 18 | 0.77 |
| (1,2945) | 1:23:A:LEU:HD21 | 1:58:A:LYS:HA | 1 | 0.77 |
| (1,2945) | 1:23:A:LEU:HD22 | 1:58:A:LYS:HA | 1 | 0.77 |
| (1,2945) | 1:23:A:LEU:HD23 | 1:58:A:LYS:HA | 1 | 0.77 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 4 | 0.77 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 8 | 0.77 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 15 | 0.77 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 15 | 0.77 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 15 | 0.77 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 12 | 0.77 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 12 | 0.77 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 12 | 0.77 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 8 | 0.77 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 8 | 0.77 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 8 | 0.77 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 12 | 0.77 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 12 | 0.77 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 12 | 0.77 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 12 | 0.77 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 12 | 0.77 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 12 | 0.77 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 12 | 0.77 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 12 | 0.77 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 12 | 0.77 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 16 | 0.77 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 16 | 0.77 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 16 | 0.77 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 16 | 0.77 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 16 | 0.77 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 16 | 0.77 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 16 | 0.77 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 16 | 0.77 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 16 | 0.77 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 2 | 0.77 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 2 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 2 | 0.77 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 2 | 0.77 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 2 | 0.77 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 2 | 0.77 |
| (1,2291) | 1:117:A:LYS:HG3 | 1:120:A:ASP:H | 18 | 0.77 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 6 | 0.77 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 8 | 0.77 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 19 | 0.77 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 6 | 0.77 |
| (1,2016) | 1:117:A:LYS:HD3 | 1:119:A:GLU:H | 8 | 0.77 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 13 | 0.77 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 13 | 0.77 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 13 | 0.77 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 15 | 0.77 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 15 | 0.77 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 15 | 0.77 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 15 | 0.77 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 15 | 0.77 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 15 | 0.77 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 18 | 0.77 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 20 | 0.77 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 20 | 0.77 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 20 | 0.77 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 1 | 0.77 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 1 | 0.77 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 1 | 0.77 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB2 | 5 | 0.77 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB3 | 5 | 0.77 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 19 | 0.77 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 9 | 0.77 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 9 | 0.77 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 9 | 0.77 |
| (1,1409) | 1:67:A:LEU:HB2 | 1:70:A:ASP:HB3 | 7 | 0.77 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 7 | 0.77 |
| (1,1351) | 1:179:A:ASP:HB2 | 1:183:A:GLN:HE21 | 4 | 0.77 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 19 | 0.77 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 19 | 0.77 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 19 | 0.77 |
| (1,1118) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HE22 | 20 | 0.77 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 3 | 0.77 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 4 | 0.77 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 11 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 11 | 0.77 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 11 | 0.77 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 18 | 0.77 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 19 | 0.77 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 19 | 0.77 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 19 | 0.77 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 18 | 0.77 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 4 | 0.77 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 4 | 0.77 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 4 | 0.77 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 10 | 0.77 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 10 | 0.77 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 10 | 0.77 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 9 | 0.77 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 12 | 0.77 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 16 | 0.77 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 16 | 0.77 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 16 | 0.77 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 7 | 0.77 |
| (1,526) | 1:172:A:VAL:HG21 | 1:176:A:GLN:H | 19 | 0.77 |
| (1,526) | 1:172:A:VAL:HG22 | 1:176:A:GLN:H | 19 | 0.77 |
| (1,526) | 1:172:A:VAL:HG23 | 1:176:A:GLN:H | 19 | 0.77 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 17 | 0.77 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 17 | 0.77 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 17 | 0.77 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 19 | 0.77 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 19 | 0.77 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 19 | 0.77 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 20 | 0.77 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 20 | 0.77 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 20 | 0.77 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 12 | 0.77 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 12 | 0.77 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 12 | 0.77 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 19 | 0.77 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 19 | 0.77 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 19 | 0.77 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 5 | 0.77 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 12 | 0.77 |
| (1,163) | 1:69:A:LYS:H | 1:70:A:ASP:HB3 | 15 | 0.77 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 8 | 0.77 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 12 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 12 | 0.77 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 12 | 0.77 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 1 | 0.76 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 1 | 0.76 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 1 | 0.76 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 1 | 0.76 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 17 | 0.76 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 17 | 0.76 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 17 | 0.76 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 17 | 0.76 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 17 | 0.76 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 17 | 0.76 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG11 | 3 | 0.76 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG12 | 3 | 0.76 |
| (1,3391) | 1:128:A:PHE:HD1 | 1:129:A:VAL:HG13 | 3 | 0.76 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 18 | 0.76 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 4 | 0.76 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD11 | 19 | 0.76 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD12 | 19 | 0.76 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD13 | 19 | 0.76 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG21 | 13 | 0.76 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG22 | 13 | 0.76 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG23 | 13 | 0.76 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG21 | 13 | 0.76 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG22 | 13 | 0.76 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG23 | 13 | 0.76 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 9 | 0.76 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 9 | 0.76 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 9 | 0.76 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 8 | 0.76 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 8 | 0.76 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 8 | 0.76 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 20 | 0.76 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 20 | 0.76 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 20 | 0.76 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 16 | 0.76 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 1 | 0.76 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 10 | 0.76 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 12 | 0.76 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 13 | 0.76 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 15 | 0.76 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 19 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 20 | 0.76 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 20 | 0.76 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 20 | 0.76 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 5 | 0.76 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 5 | 0.76 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 5 | 0.76 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 16 | 0.76 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 16 | 0.76 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 16 | 0.76 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 16 | 0.76 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 16 | 0.76 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 16 | 0.76 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 2 | 0.76 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 2 | 0.76 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 2 | 0.76 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 6 | 0.76 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 6 | 0.76 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 6 | 0.76 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG12 | 7 | 0.76 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG13 | 7 | 0.76 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 2 | 0.76 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG21 | 20 | 0.76 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG22 | 20 | 0.76 |
| (1,1454) | 1:45:A:ASN:HB3 | 1:174:A:VAL:HG23 | 20 | 0.76 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG11 | 9 | 0.76 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG12 | 9 | 0.76 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG13 | 9 | 0.76 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 20 | 0.76 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 20 | 0.76 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 20 | 0.76 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 16 | 0.76 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 16 | 0.76 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 16 | 0.76 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 1 | 0.76 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 1 | 0.76 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 1 | 0.76 |
| (1,1409) | 1:67:A:LEU:HB2 | 1:70:A:ASP:HB3 | 2 | 0.76 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 4 | 0.76 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 5 | 0.76 |
| (1,1351) | 1:179:A:ASP:HB2 | 1:183:A:GLN:HE21 | 15 | 0.76 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 2 | 0.76 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 4 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 4 | 0.76 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 4 | 0.76 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 13 | 0.76 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 13 | 0.76 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 13 | 0.76 |
| (1,979) | 1:29:A:TYR:H | 1:71:A:LEU:HD11 | 10 | 0.76 |
| (1,979) | 1:29:A:TYR:H | 1:71:A:LEU:HD12 | 10 | 0.76 |
| (1,979) | 1:29:A:TYR:H | 1:71:A:LEU:HD13 | 10 | 0.76 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 18 | 0.76 |
| (1,883) | 1:49:A:LYS:H | 1:49:A:LYS:HD3 | 10 | 0.76 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 14 | 0.76 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 14 | 0.76 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 14 | 0.76 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 16 | 0.76 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 16 | 0.76 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 16 | 0.76 |
| (1,683) | 1:168:A:SER:H | 1:170:A:MET:HG2 | 20 | 0.76 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 18 | 0.76 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 9 | 0.76 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 9 | 0.76 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 9 | 0.76 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 10 | 0.76 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 10 | 0.76 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 10 | 0.76 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 17 | 0.76 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 5 | 0.75 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 5 | 0.75 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE1 | 5 | 0.75 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE2 | 5 | 0.75 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE1 | 14 | 0.75 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE2 | 14 | 0.75 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE1 | 15 | 0.75 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE2 | 15 | 0.75 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 7 | 0.75 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 7 | 0.75 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 7 | 0.75 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 7 | 0.75 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 7 | 0.75 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 7 | 0.75 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 12 | 0.75 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 19 | 0.75 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 19 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 19 | 0.75 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 19 | 0.75 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 19 | 0.75 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 19 | 0.75 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 20 | 0.75 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 17 | 0.75 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 17 | 0.75 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 17 | 0.75 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 15 | 0.75 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 15 | 0.75 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 15 | 0.75 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 19 | 0.75 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 19 | 0.75 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 19 | 0.75 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 16 | 0.75 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 16 | 0.75 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 16 | 0.75 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 4 | 0.75 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 4 | 0.75 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 4 | 0.75 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 16 | 0.75 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 16 | 0.75 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 16 | 0.75 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 16 | 0.75 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 16 | 0.75 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 16 | 0.75 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 16 | 0.75 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 16 | 0.75 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 16 | 0.75 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 4 | 0.75 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 19 | 0.75 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 19 | 0.75 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 19 | 0.75 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 14 | 0.75 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 1 | 0.75 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 6 | 0.75 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 14 | 0.75 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 17 | 0.75 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 19 | 0.75 |
| (1,2332) | 1:3:A:ILE:HA | 1:7:A:LYS:HB2 | 17 | 0.75 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 14 | 0.75 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 14 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 14 | 0.75 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 14 | 0.75 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 14 | 0.75 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 14 | 0.75 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 18 | 0.75 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 18 | 0.75 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 18 | 0.75 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 18 | 0.75 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 18 | 0.75 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 18 | 0.75 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 9 | 0.75 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 20 | 0.75 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 4 | 0.75 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 19 | 0.75 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG11 | 8 | 0.75 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG12 | 8 | 0.75 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG13 | 8 | 0.75 |
| (1,2017) | 1:117:A:LYS:HD3 | 1:120:A:ASP:H | 1 | 0.75 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 18 | 0.75 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG12 | 8 | 0.75 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG13 | 8 | 0.75 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 2 | 0.75 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 3 | 0.75 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 3 | 0.75 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 3 | 0.75 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 12 | 0.75 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 2 | 0.75 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 13 | 0.75 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 17 | 0.75 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 17 | 0.75 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 17 | 0.75 |
| (1,1444) | 1:83:A:VAL:HA | 1:85:A:ASP:HB2 | 8 | 0.75 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 5 | 0.75 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 5 | 0.75 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 5 | 0.75 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 17 | 0.75 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 17 | 0.75 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 17 | 0.75 |
| (1,1409) | 1:67:A:LEU:HB2 | 1:70:A:ASP:HB3 | 10 | 0.75 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 14 | 0.75 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 20 | 0.75 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 20 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 20 | 0.75 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 1 | 0.75 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 1 | 0.75 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 1 | 0.75 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 20 | 0.75 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 20 | 0.75 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 20 | 0.75 |
| (1,991) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HD22 | 10 | 0.75 |
| (1,991) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HD22 | 19 | 0.75 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 9 | 0.75 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 12 | 0.75 |
| (1,904) | 1:127:A:SER:H | 1:127:A:SER:HB3 | 7 | 0.75 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 16 | 0.75 |
| (1,894) | 1:103:A:SER:H | 1:106:A:ASP:HB3 | 15 | 0.75 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 2 | 0.75 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 2 | 0.75 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 2 | 0.75 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD21 | 11 | 0.75 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD22 | 11 | 0.75 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD23 | 11 | 0.75 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 15 | 0.75 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 10 | 0.75 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 10 | 0.75 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 10 | 0.75 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 1 | 0.75 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 1 | 0.75 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 1 | 0.75 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 10 | 0.75 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 10 | 0.75 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 10 | 0.75 |
| (1,628) | 1:90:A:PRO:HB3 | 1:91:A:MET:H | 19 | 0.75 |
| (1,553) | 1:42:A:VAL:HG21 | 1:46:A:VAL:H | 16 | 0.75 |
| (1,553) | 1:42:A:VAL:HG22 | 1:46:A:VAL:H | 16 | 0.75 |
| (1,553) | 1:42:A:VAL:HG23 | 1:46:A:VAL:H | 16 | 0.75 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 9 | 0.75 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 9 | 0.75 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 9 | 0.75 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 4 | 0.75 |
| (1,128) | 1:12:A:LEU:HD11 | 1:159:A:GLN:H | 16 | 0.75 |
| (1,128) | 1:12:A:LEU:HD12 | 1:159:A:GLN:H | 16 | 0.75 |
| (1,128) | 1:12:A:LEU:HD13 | 1:159:A:GLN:H | 16 | 0.75 |
| (1,90) | 1:185:A:VAL:HA | 1:188:A:LYS:H | 18 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 2 | 0.74 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 16 | 0.74 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 16 | 0.74 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 16 | 0.74 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 16 | 0.74 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 16 | 0.74 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 16 | 0.74 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB2 | 1 | 0.74 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB3 | 1 | 0.74 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB2 | 1 | 0.74 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB3 | 1 | 0.74 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 8 | 0.74 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 10 | 0.74 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 17 | 0.74 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 17 | 0.74 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 4 | 0.74 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 17 | 0.74 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 13 | 0.74 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 13 | 0.74 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 13 | 0.74 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 15 | 0.74 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 15 | 0.74 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 15 | 0.74 |
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 20 | 0.74 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 1 | 0.74 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 1 | 0.74 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 1 | 0.74 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 4 | 0.74 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 4 | 0.74 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 4 | 0.74 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 3 | 0.74 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 3 | 0.74 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 3 | 0.74 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 14 | 0.74 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 14 | 0.74 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 14 | 0.74 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 12 | 0.74 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 12 | 0.74 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 12 | 0.74 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 6 | 0.74 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 6 | 0.74 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 6 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 8 | 0.74 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 12 | 0.74 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 13 | 0.74 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 6 | 0.74 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 8 | 0.74 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 8 | 0.74 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 8 | 0.74 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 10 | 0.74 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 20 | 0.74 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG11 | 1 | 0.74 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG12 | 1 | 0.74 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG13 | 1 | 0.74 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 9 | 0.74 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 9 | 0.74 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 9 | 0.74 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 15 | 0.74 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 15 | 0.74 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 15 | 0.74 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 14 | 0.74 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 14 | 0.74 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 14 | 0.74 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 12 | 0.74 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 12 | 0.74 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 20 | 0.74 |
| (1,1354) | 1:73:A:GLN:HE22 | 1:131:A:LYS:HE2 | 18 | 0.74 |
| (1,1354) | 1:73:A:GLN:HE22 | 1:131:A:LYS:HE3 | 18 | 0.74 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 17 | 0.74 |
| (1,1258) | 1:163:A:GLN:HG2 | 1:164:A:GLY:HA3 | 18 | 0.74 |
| (1,1258) | 1:163:A:GLN:HG3 | 1:164:A:GLY:HA3 | 18 | 0.74 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG11 | 3 | 0.74 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG12 | 3 | 0.74 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG13 | 3 | 0.74 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 2 | 0.74 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 10 | 0.74 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 1 | 0.74 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 1 | 0.74 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 19 | 0.74 |
| (1,683) | 1:168:A:SER:H | 1:170:A:MET:HG2 | 13 | 0.74 |
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 19 | 0.74 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 13 | 0.74 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 6 | 0.74 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 15 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 6 | 0.74 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 6 | 0.74 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 6 | 0.74 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 19 | 0.74 |
| (1,163) | 1:69:A:LYS:H | 1:70:A:ASP:HB3 | 2 | 0.74 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 16 | 0.74 |
| (1,127) | 1:105:A:ALA:H | 1:107:A:ILE:HB | 9 | 0.74 |
| (1,111) | 1:103:A:SER:HB2 | 1:105:A:ALA:H | 20 | 0.74 |
| (1,3495) | 1:23:A:LEU:HD21 | 1:59:A:TYR:HE1 | 14 | 0.73 |
| (1,3495) | 1:23:A:LEU:HD21 | 1:59:A:TYR:HE2 | 14 | 0.73 |
| (1,3495) | 1:23:A:LEU:HD22 | 1:59:A:TYR:HE1 | 14 | 0.73 |
| (1,3495) | 1:23:A:LEU:HD22 | 1:59:A:TYR:HE2 | 14 | 0.73 |
| (1,3495) | 1:23:A:LEU:HD23 | 1:59:A:TYR:HE1 | 14 | 0.73 |
| (1,3495) | 1:23:A:LEU:HD23 | 1:59:A:TYR:HE2 | 14 | 0.73 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 11 | 0.73 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 11 | 0.73 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 11 | 0.73 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 11 | 0.73 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 11 | 0.73 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 11 | 0.73 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 18 | 0.73 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 18 | 0.73 |
| (1,3171) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HB2 | 7 | 0.73 |
| (1,3171) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HB2 | 7 | 0.73 |
| (1,3171) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HB2 | 7 | 0.73 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE1 | 17 | 0.73 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE2 | 17 | 0.73 |
| (1,3133) | 1:152:A:MET:HB2 | 1:152:A:MET:HE3 | 17 | 0.73 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 3 | 0.73 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 3 | 0.73 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 3 | 0.73 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 3 | 0.73 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 3 | 0.73 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 3 | 0.73 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 3 | 0.73 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 3 | 0.73 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 3 | 0.73 |
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 3 | 0.73 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 3 | 0.73 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 3 | 0.73 |
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 14 | 0.73 |
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 5 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 2 | 0.73 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 11 | 0.73 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 11 | 0.73 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 11 | 0.73 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 11 | 0.73 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 11 | 0.73 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 11 | 0.73 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 11 | 0.73 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 11 | 0.73 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 11 | 0.73 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 3 | 0.73 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 3 | 0.73 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 3 | 0.73 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 3 | 0.73 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 3 | 0.73 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 3 | 0.73 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 11 | 0.73 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 11 | 0.73 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 11 | 0.73 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 20 | 0.73 |
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 2 | 0.73 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 2 | 0.73 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 2 | 0.73 |
| (1,2425) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HA | 7 | 0.73 |
| (1,2425) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HA | 7 | 0.73 |
| (1,2425) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HA | 7 | 0.73 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 2 | 0.73 |
| (1,2168) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HG2 | 10 | 0.73 |
| (1,2168) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HG2 | 10 | 0.73 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 9 | 0.73 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD1 | 3 | 0.73 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD2 | 3 | 0.73 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 3 | 0.73 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 8 | 0.73 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 8 | 0.73 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 8 | 0.73 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG21 | 5 | 0.73 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG22 | 5 | 0.73 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG23 | 5 | 0.73 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 4 | 0.73 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 4 | 0.73 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 4 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 11 | 0.73 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 11 | 0.73 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 11 | 0.73 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 10 | 0.73 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 20 | 0.73 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 10 | 0.73 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 10 | 0.73 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 10 | 0.73 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 8 | 0.73 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 8 | 0.73 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 12 | 0.73 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 12 | 0.73 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 12 | 0.73 |
| (1,1409) | 1:67:A:LEU:HB2 | 1:70:A:ASP:HB3 | 14 | 0.73 |
| (1,1409) | 1:67:A:LEU:HB2 | 1:70:A:ASP:HB3 | 17 | 0.73 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 17 | 0.73 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 13 | 0.73 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 18 | 0.73 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 18 | 0.73 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 18 | 0.73 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 1 | 0.73 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 1 | 0.73 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 1 | 0.73 |
| (1,899) | 1:67:A:LEU:HD21 | 1:103:A:SER:H | 3 | 0.73 |
| (1,899) | 1:67:A:LEU:HD22 | 1:103:A:SER:H | 3 | 0.73 |
| (1,899) | 1:67:A:LEU:HD23 | 1:103:A:SER:H | 3 | 0.73 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 5 | 0.73 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 20 | 0.73 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 6 | 0.73 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 6 | 0.73 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 6 | 0.73 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 17 | 0.73 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 17 | 0.73 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 17 | 0.73 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 16 | 0.73 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 16 | 0.73 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 19 | 0.73 |
| (1,441) | 1:34:A:TYR:HE2 | 1:92:A:PHE:H | 12 | 0.73 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 1 | 0.73 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 1 | 0.73 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 1 | 0.73 |
| (1,242) | 1:145:A:GLN:HE21 | 1:147:A:GLN:H | 11 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 6 | 0.72 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 6 | 0.72 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 7 | 0.72 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 14 | 0.72 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 6 | 0.72 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 6 | 0.72 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 17 | 0.72 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 17 | 0.72 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 18 | 0.72 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 18 | 0.72 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 18 | 0.72 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 18 | 0.72 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 18 | 0.72 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 18 | 0.72 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 8 | 0.72 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 15 | 0.72 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 16 | 0.72 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 8 | 0.72 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 8 | 0.72 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 8 | 0.72 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE1 | 3 | 0.72 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE2 | 3 | 0.72 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE3 | 3 | 0.72 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 7 | 0.72 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 7 | 0.72 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 7 | 0.72 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 7 | 0.72 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 7 | 0.72 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 7 | 0.72 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 7 | 0.72 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 7 | 0.72 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 7 | 0.72 |
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 11 | 0.72 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 8 | 0.72 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 8 | 0.72 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 8 | 0.72 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 17 | 0.72 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 17 | 0.72 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 17 | 0.72 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 12 | 0.72 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 12 | 0.72 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 12 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2437) | 1:181:A:VAL:HG21 | 1:184:A:LEU:H | 7 | 0.72 |
| (1,2437) | 1:181:A:VAL:HG22 | 1:184:A:LEU:H | 7 | 0.72 |
| (1,2437) | 1:181:A:VAL:HG23 | 1:184:A:LEU:H | 7 | 0.72 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 3 | 0.72 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 19 | 0.72 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 19 | 0.72 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 19 | 0.72 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 3 | 0.72 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 3 | 0.72 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 3 | 0.72 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 3 | 0.72 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 3 | 0.72 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 3 | 0.72 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 15 | 0.72 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 15 | 0.72 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 15 | 0.72 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 15 | 0.72 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 15 | 0.72 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 15 | 0.72 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 10 | 0.72 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 1 | 0.72 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 7 | 0.72 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 14 | 0.72 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 19 | 0.72 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 13 | 0.72 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 13 | 0.72 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 13 | 0.72 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 5 | 0.72 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 5 | 0.72 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 5 | 0.72 |
| (1,1931) | 1:62:A:GLU:HB2 | 1:63:A:PHE:HB3 | 3 | 0.72 |
| (1,1931) | 1:62:A:GLU:HB3 | 1:63:A:PHE:HB3 | 3 | 0.72 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 9 | 0.72 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 9 | 0.72 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 9 | 0.72 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 9 | 0.72 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 9 | 0.72 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 9 | 0.72 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 11 | 0.72 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 11 | 0.72 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 11 | 0.72 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 2 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 2 | 0.72 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 2 | 0.72 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 4 | 0.72 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 4 | 0.72 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 4 | 0.72 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 14 | 0.72 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 19 | 0.72 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 11 | 0.72 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 20 | 0.72 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG11 | 7 | 0.72 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG12 | 7 | 0.72 |
| (1,921) | 1:37:A:GLU:H | 1:39:A:VAL:HG13 | 7 | 0.72 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 6 | 0.72 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 9 | 0.72 |
| (1,894) | 1:103:A:SER:H | 1:106:A:ASP:HB3 | 2 | 0.72 |
| (1,894) | 1:103:A:SER:H | 1:106:A:ASP:HB3 | 4 | 0.72 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 4 | 0.72 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 4 | 0.72 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 4 | 0.72 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 16 | 0.72 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 16 | 0.72 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 16 | 0.72 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 8 | 0.72 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 8 | 0.72 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 8 | 0.72 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG21 | 13 | 0.72 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG22 | 13 | 0.72 |
| (1,706) | 1:45:A:ASN:H | 1:174:A:VAL:HG23 | 13 | 0.72 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 2 | 0.72 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 2 | 0.72 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 2 | 0.72 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 9 | 0.72 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 9 | 0.72 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 9 | 0.72 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 13 | 0.72 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 13 | 0.72 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 13 | 0.72 |
| (1,90) | 1:185:A:VAL:HA | 1:188:A:LYS:H | 12 | 0.72 |
| (1,90) | 1:185:A:VAL:HA | 1:188:A:LYS:H | 16 | 0.72 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 10 | 0.71 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 10 | 0.71 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 7 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 7 | 0.71 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 7 | 0.71 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 7 | 0.71 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 7 | 0.71 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 7 | 0.71 |
| (1,3494) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HG3 | 6 | 0.71 |
| (1,3494) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HG3 | 6 | 0.71 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB2 | 10 | 0.71 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB3 | 10 | 0.71 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB2 | 10 | 0.71 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB3 | 10 | 0.71 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD1 | 16 | 0.71 |
| (1,3346) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HD2 | 16 | 0.71 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD1 | 16 | 0.71 |
| (1,3346) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HD2 | 16 | 0.71 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD1 | 16 | 0.71 |
| (1,3346) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HD2 | 16 | 0.71 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 15 | 0.71 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 19 | 0.71 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG21 | 6 | 0.71 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG22 | 6 | 0.71 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG23 | 6 | 0.71 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG21 | 6 | 0.71 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG22 | 6 | 0.71 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG23 | 6 | 0.71 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG21 | 6 | 0.71 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG22 | 6 | 0.71 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG23 | 6 | 0.71 |
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 15 | 0.71 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 6 | 0.71 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 6 | 0.71 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 6 | 0.71 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 10 | 0.71 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 10 | 0.71 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 10 | 0.71 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 4 | 0.71 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 4 | 0.71 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 4 | 0.71 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG11 | 11 | 0.71 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG12 | 11 | 0.71 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG13 | 11 | 0.71 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD21 | 1 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD22 | 1 | 0.71 |
| (1,2426) | 1:47:A:ARG:HA | 1:50:A:LEU:HD23 | 1 | 0.71 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 13 | 0.71 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 15 | 0.71 |
| (1,2345) | 1:7:A:LYS:HG3 | 1:8:A:GLN:HB2 | 3 | 0.71 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 7 | 0.71 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 20 | 0.71 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 20 | 0.71 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 20 | 0.71 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 14 | 0.71 |
| (1,2013) | 1:117:A:LYS:HD3 | 1:118:A:GLY:H | 11 | 0.71 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG21 | 14 | 0.71 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG22 | 14 | 0.71 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG23 | 14 | 0.71 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 15 | 0.71 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 15 | 0.71 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 15 | 0.71 |
| (1,1778) | 1:72:A:THR:HB | 1:73:A:GLN:HB3 | 20 | 0.71 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 20 | 0.71 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 20 | 0.71 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 20 | 0.71 |
| (1,1577) | 1:152:A:MET:HB3 | 1:160:A:LEU:HB2 | 1 | 0.71 |
| (1,1577) | 1:152:A:MET:HB3 | 1:160:A:LEU:HB2 | 17 | 0.71 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 5 | 0.71 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 5 | 0.71 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 5 | 0.71 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 6 | 0.71 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 6 | 0.71 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 6 | 0.71 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 6 | 0.71 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 20 | 0.71 |
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 20 | 0.71 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 20 | 0.71 |
| (1,1426) | 1:143:A:ASP:HB2 | 1:144:A:LEU:HG | 19 | 0.71 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 20 | 0.71 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 20 | 0.71 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 20 | 0.71 |
| (1,1358) | 1:179:A:ASP:HB3 | 1:183:A:GLN:HE21 | 10 | 0.71 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 10 | 0.71 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 10 | 0.71 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 10 | 0.71 |
| (1,1058) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HA | 8 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,937) | 1:116:A:VAL:HG21 | 1:118:A:GLY:H | 4 | 0.71 |
| (1,937) | 1:116:A:VAL:HG22 | 1:118:A:GLY:H | 4 | 0.71 |
| (1,937) | 1:116:A:VAL:HG23 | 1:118:A:GLY:H | 4 | 0.71 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 10 | 0.71 |
| (1,894) | 1:103:A:SER:H | 1:106:A:ASP:HB3 | 12 | 0.71 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 4 | 0.71 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 6 | 0.71 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 13 | 0.71 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 4 | 0.71 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 6 | 0.71 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 6 | 0.71 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 6 | 0.71 |
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 3 | 0.71 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 7 | 0.71 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 7 | 0.71 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 7 | 0.71 |
| (1,353) | 1:108:A:ARG:HG3 | 1:112:A:VAL:H | 7 | 0.71 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 19 | 0.71 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 19 | 0.71 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 19 | 0.71 |
| (1,163) | 1:69:A:LYS:H | 1:70:A:ASP:HB3 | 10 | 0.71 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 18 | 0.71 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 18 | 0.71 |
| (1,128) | 1:12:A:LEU:HD11 | 1:159:A:GLN:H | 11 | 0.71 |
| (1,128) | 1:12:A:LEU:HD12 | 1:159:A:GLN:H | 11 | 0.71 |
| (1,128) | 1:12:A:LEU:HD13 | 1:159:A:GLN:H | 11 | 0.71 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 10 | 0.7 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 10 | 0.7 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 10 | 0.7 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 10 | 0.7 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 11 | 0.7 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 11 | 0.7 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 9 | 0.7 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 9 | 0.7 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 18 | 0.7 |
| (1,3442) | 1:73:A:GLN:HG2 | 1:125:A:TRP:HH2 | 13 | 0.7 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 4 | 0.7 |
| (1,3311) | 1:29:A:TYR:HD1 | 1:71:A:LEU:HB2 | 17 | 0.7 |
| (1,3311) | 1:29:A:TYR:HD2 | 1:71:A:LEU:HB2 | 17 | 0.7 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 1 | 0.7 |
| (1,3112) | 1:67:A:LEU:HA | 1:70:A:ASP:HB3 | 7 | 0.7 |
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 9 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 7 | 0.7 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 7 | 0.7 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 7 | 0.7 |
| (1,2838) | 1:34:A:TYR:HE1 | 1:38:A:GLU:HA | 14 | 0.7 |
| (1,2838) | 1:34:A:TYR:HE2 | 1:38:A:GLU:HA | 14 | 0.7 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 2 | 0.7 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 2 | 0.7 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 2 | 0.7 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 15 | 0.7 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 15 | 0.7 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 15 | 0.7 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG11 | 20 | 0.7 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG12 | 20 | 0.7 |
| (1,2662) | 1:171:A:ASP:HA | 1:174:A:VAL:HG13 | 20 | 0.7 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 7 | 0.7 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 7 | 0.7 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 7 | 0.7 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 20 | 0.7 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 20 | 0.7 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 20 | 0.7 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 3 | 0.7 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 3 | 0.7 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 3 | 0.7 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 3 | 0.7 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 3 | 0.7 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 3 | 0.7 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 3 | 0.7 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 3 | 0.7 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 3 | 0.7 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 4 | 0.7 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 18 | 0.7 |
| (1,2316) | 1:117:A:LYS:H | 1:117:A:LYS:HG2 | 18 | 0.7 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 2 | 0.7 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD1 | 9 | 0.7 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD2 | 9 | 0.7 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 3 | 0.7 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 20 | 0.7 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 5 | 0.7 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 8 | 0.7 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 8 | 0.7 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 8 | 0.7 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 10 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 10 | 0.7 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 10 | 0.7 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 20 | 0.7 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB2 | 14 | 0.7 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB3 | 14 | 0.7 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 14 | 0.7 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 14 | 0.7 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 14 | 0.7 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 15 | 0.7 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 17 | 0.7 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 2 | 0.7 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 3 | 0.7 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 5 | 0.7 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 8 | 0.7 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 8 | 0.7 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 8 | 0.7 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 11 | 0.7 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 19 | 0.7 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 19 | 0.7 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 19 | 0.7 |
| (1,778) | 1:51:A:PRO:HB3 | 1:54:A:THR:H | 4 | 0.7 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 4 | 0.7 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 9 | 0.7 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 9 | 0.7 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 9 | 0.7 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 8 | 0.7 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 14 | 0.7 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 1 | 0.7 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 5 | 0.7 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 10 | 0.7 |
| (1,441) | 1:34:A:TYR:HD2 | 1:92:A:PHE:H | 8 | 0.7 |
| (1,416) | 1:122:A:ASP:HB3 | 1:123:A:ALA:H | 8 | 0.7 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 10 | 0.7 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 10 | 0.7 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 10 | 0.7 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 12 | 0.7 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 12 | 0.7 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 12 | 0.7 |
| (1,163) | 1:69:A:LYS:H | 1:70:A:ASP:HB3 | 20 | 0.7 |
| (1,128) | 1:12:A:LEU:HD11 | 1:159:A:GLN:H | 17 | 0.7 |
| (1,128) | 1:12:A:LEU:HD12 | 1:159:A:GLN:H | 17 | 0.7 |
| (1,128) | 1:12:A:LEU:HD13 | 1:159:A:GLN:H | 17 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 3 | 0.69 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 16 | 0.69 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 16 | 0.69 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 16 | 0.69 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 16 | 0.69 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 9 | 0.69 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 9 | 0.69 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 9 | 0.69 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 9 | 0.69 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 9 | 0.69 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 9 | 0.69 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 2 | 0.69 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 17 | 0.69 |
| (1,3269) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA2 | 13 | 0.69 |
| (1,3269) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA2 | 13 | 0.69 |
| (1,3269) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA2 | 13 | 0.69 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG21 | 7 | 0.69 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG22 | 7 | 0.69 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG23 | 7 | 0.69 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG21 | 7 | 0.69 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG22 | 7 | 0.69 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG23 | 7 | 0.69 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG21 | 7 | 0.69 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG22 | 7 | 0.69 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG23 | 7 | 0.69 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE1 | 8 | 0.69 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE2 | 8 | 0.69 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE3 | 8 | 0.69 |
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 2 | 0.69 |
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 17 | 0.69 |
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 4 | 0.69 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 8 | 0.69 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 8 | 0.69 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 8 | 0.69 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 4 | 0.69 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 4 | 0.69 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 4 | 0.69 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG21 | 17 | 0.69 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG22 | 17 | 0.69 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG23 | 17 | 0.69 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG21 | 17 | 0.69 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG22 | 17 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG23 | 17 | 0.69 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 1 | 0.69 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 1 | 0.69 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 1 | 0.69 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 11 | 0.69 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 11 | 0.69 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 11 | 0.69 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 11 | 0.69 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 11 | 0.69 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 11 | 0.69 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 11 | 0.69 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 11 | 0.69 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 11 | 0.69 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 14 | 0.69 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 14 | 0.69 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 14 | 0.69 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 14 | 0.69 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 14 | 0.69 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 14 | 0.69 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 14 | 0.69 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 14 | 0.69 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 14 | 0.69 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 16 | 0.69 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 13 | 0.69 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 11 | 0.69 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 16 | 0.69 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 16 | 0.69 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 16 | 0.69 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 13 | 0.69 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 13 | 0.69 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 13 | 0.69 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 13 | 0.69 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 13 | 0.69 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 13 | 0.69 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 16 | 0.69 |
| (1,2016) | 1:117:A:LYS:HD3 | 1:119:A:GLU:H | 9 | 0.69 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 13 | 0.69 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 9 | 0.69 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 9 | 0.69 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 9 | 0.69 |
| (1,1697) | 1:132:A:SER:HB2 | 1:136:A:GLN:HG2 | 14 | 0.69 |
| (1,1697) | 1:132:A:SER:HB3 | 1:136:A:GLN:HG2 | 14 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 6 | 0.69 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 10 | 0.69 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 10 | 0.69 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 10 | 0.69 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB2 | 18 | 0.69 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB3 | 18 | 0.69 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 9 | 0.69 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 9 | 0.69 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 9 | 0.69 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 1 | 0.69 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 6 | 0.69 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 12 | 0.69 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 13 | 0.69 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 15 | 0.69 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 15 | 0.69 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 15 | 0.69 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 2 | 0.69 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 9 | 0.69 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 2 | 0.69 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 4 | 0.69 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 12 | 0.69 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 12 | 0.69 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 12 | 0.69 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 8 | 0.69 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 5 | 0.69 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 5 | 0.69 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 5 | 0.69 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 14 | 0.69 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 14 | 0.69 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 14 | 0.69 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 9 | 0.69 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 10 | 0.69 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 4 | 0.69 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 8 | 0.69 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 8 | 0.69 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 8 | 0.69 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 12 | 0.69 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 14 | 0.69 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 14 | 0.69 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 14 | 0.69 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 15 | 0.69 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 16 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 6 | 0.69 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 6 | 0.69 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 6 | 0.69 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 1 | 0.69 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 7 | 0.69 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 1 | 0.69 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 11 | 0.69 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 5 | 0.69 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 6 | 0.69 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 18 | 0.69 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 13 | 0.68 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 13 | 0.68 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 14 | 0.68 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 14 | 0.68 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 14 | 0.68 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 14 | 0.68 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 14 | 0.68 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 14 | 0.68 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 15 | 0.68 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 15 | 0.68 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 15 | 0.68 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 4 | 0.68 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 4 | 0.68 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 4 | 0.68 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 4 | 0.68 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 4 | 0.68 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 4 | 0.68 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE1 | 12 | 0.68 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE2 | 12 | 0.68 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE3 | 12 | 0.68 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG21 | 5 | 0.68 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG22 | 5 | 0.68 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG23 | 5 | 0.68 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG21 | 5 | 0.68 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG22 | 5 | 0.68 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG23 | 5 | 0.68 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG21 | 5 | 0.68 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG22 | 5 | 0.68 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG23 | 5 | 0.68 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG21 | 5 | 0.68 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG22 | 5 | 0.68 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG23 | 5 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG21 | 5 | 0.68 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG22 | 5 | 0.68 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG23 | 5 | 0.68 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG21 | 5 | 0.68 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG22 | 5 | 0.68 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG23 | 5 | 0.68 |
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 7 | 0.68 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG11 | 7 | 0.68 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG12 | 7 | 0.68 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG13 | 7 | 0.68 |
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 13 | 0.68 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 13 | 0.68 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 13 | 0.68 |
| (1,2927) | 1:58:A:LYS:HA | 1:59:A:TYR:HB3 | 7 | 0.68 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 19 | 0.68 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 19 | 0.68 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 19 | 0.68 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 19 | 0.68 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 19 | 0.68 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 19 | 0.68 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 19 | 0.68 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 19 | 0.68 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 19 | 0.68 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 8 | 0.68 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 8 | 0.68 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 8 | 0.68 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 19 | 0.68 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 19 | 0.68 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 19 | 0.68 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 9 | 0.68 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 9 | 0.68 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 9 | 0.68 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 6 | 0.68 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 6 | 0.68 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 6 | 0.68 |
| (1,2555) | 1:40:A:LEU:HD21 | 1:170:A:MET:HG3 | 18 | 0.68 |
| (1,2555) | 1:40:A:LEU:HD22 | 1:170:A:MET:HG3 | 18 | 0.68 |
| (1,2555) | 1:40:A:LEU:HD23 | 1:170:A:MET:HG3 | 18 | 0.68 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 17 | 0.68 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 17 | 0.68 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 17 | 0.68 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 12 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 12 | 0.68 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 12 | 0.68 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 12 | 0.68 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 12 | 0.68 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 12 | 0.68 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 12 | 0.68 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 12 | 0.68 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 12 | 0.68 |
| (1,2392) | 1:31:A:PRO:HA | 1:34:A:TYR:HA | 18 | 0.68 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 17 | 0.68 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 11 | 0.68 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 11 | 0.68 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 11 | 0.68 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 11 | 0.68 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 11 | 0.68 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 11 | 0.68 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 13 | 0.68 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 15 | 0.68 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 10 | 0.68 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD21 | 7 | 0.68 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD22 | 7 | 0.68 |
| (1,1817) | 1:181:A:VAL:HA | 1:184:A:LEU:HD23 | 7 | 0.68 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 20 | 0.68 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 20 | 0.68 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 20 | 0.68 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 20 | 0.68 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 20 | 0.68 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 20 | 0.68 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG12 | 16 | 0.68 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG13 | 16 | 0.68 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 1 | 0.68 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 1 | 0.68 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 16 | 0.68 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 11 | 0.68 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 11 | 0.68 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 11 | 0.68 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 8 | 0.68 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 8 | 0.68 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 8 | 0.68 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 10 | 0.68 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 9 | 0.68 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 13 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 20 | 0.68 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 20 | 0.68 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 20 | 0.68 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 16 | 0.68 |
| (1,894) | 1:103:A:SER:H | 1:106:A:ASP:HB3 | 20 | 0.68 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 15 | 0.68 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 15 | 0.68 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 15 | 0.68 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 15 | 0.68 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 17 | 0.68 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 20 | 0.68 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 5 | 0.68 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 5 | 0.68 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 5 | 0.68 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 20 | 0.68 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 20 | 0.68 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 20 | 0.68 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 2 | 0.68 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 14 | 0.68 |
| (1,683) | 1:168:A:SER:H | 1:170:A:MET:HG2 | 12 | 0.68 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 3 | 0.68 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 9 | 0.68 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 20 | 0.68 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 15 | 0.68 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 15 | 0.68 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 15 | 0.68 |
| (1,337) | 1:166:A:ASP:H | 1:176:A:GLN:HE21 | 2 | 0.68 |
| (1,337) | 1:166:A:ASP:H | 1:176:A:GLN:HE21 | 20 | 0.68 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 13 | 0.68 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 13 | 0.68 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 13 | 0.68 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 3 | 0.68 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 3 | 0.68 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 3 | 0.68 |
| (1,90) | 1:185:A:VAL:HA | 1:188:A:LYS:H | 9 | 0.68 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 11 | 0.67 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 11 | 0.67 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 7 | 0.67 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 7 | 0.67 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 18 | 0.67 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 7 | 0.67 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 7 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD11 | 2 | 0.67 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD12 | 2 | 0.67 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD13 | 2 | 0.67 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD11 | 2 | 0.67 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD12 | 2 | 0.67 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD13 | 2 | 0.67 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 20 | 0.67 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 20 | 0.67 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 3 | 0.67 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 11 | 0.67 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 11 | 0.67 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 11 | 0.67 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE1 | 14 | 0.67 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE2 | 14 | 0.67 |
| (1,3072) | 1:43:A:SER:HA | 1:56:A:MET:HE3 | 14 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 11 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 11 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 11 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 11 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 11 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 11 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 11 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 11 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 11 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG21 | 12 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG22 | 12 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB1 | 1:129:A:VAL:HG23 | 12 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG21 | 12 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG22 | 12 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB2 | 1:129:A:VAL:HG23 | 12 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG21 | 12 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG22 | 12 | 0.67 |
| (1,3029) | 1:80:A:ALA:HB3 | 1:129:A:VAL:HG23 | 12 | 0.67 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 1 | 0.67 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 1 | 0.67 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 1 | 0.67 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 1 | 0.67 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 1 | 0.67 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 1 | 0.67 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 1 | 0.67 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 1 | 0.67 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 1 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 1 | 0.67 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 1 | 0.67 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 1 | 0.67 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD11 | 6 | 0.67 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD12 | 6 | 0.67 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD13 | 6 | 0.67 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 9 | 0.67 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 9 | 0.67 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 9 | 0.67 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG21 | 6 | 0.67 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG22 | 6 | 0.67 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG23 | 6 | 0.67 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG21 | 6 | 0.67 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG22 | 6 | 0.67 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG23 | 6 | 0.67 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 15 | 0.67 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 15 | 0.67 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 15 | 0.67 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 6 | 0.67 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 17 | 0.67 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 7 | 0.67 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 7 | 0.67 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 7 | 0.67 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 11 | 0.67 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 18 | 0.67 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 4 | 0.67 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 4 | 0.67 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 4 | 0.67 |
| (1,2316) | 1:117:A:LYS:H | 1:117:A:LYS:HG2 | 12 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 10 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 10 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 10 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 10 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 10 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 10 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 16 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 16 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 16 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 16 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 16 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 16 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 17 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 17 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 17 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 17 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 17 | 0.67 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 17 | 0.67 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 7 | 0.67 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 4 | 0.67 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 6 | 0.67 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 14 | 0.67 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 6 | 0.67 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 6 | 0.67 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 6 | 0.67 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 6 | 0.67 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 6 | 0.67 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 6 | 0.67 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG2 | 2 | 0.67 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG3 | 2 | 0.67 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG2 | 9 | 0.67 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG3 | 9 | 0.67 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 15 | 0.67 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 6 | 0.67 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 6 | 0.67 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 6 | 0.67 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 6 | 0.67 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 6 | 0.67 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 13 | 0.67 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 13 | 0.67 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 13 | 0.67 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 16 | 0.67 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 16 | 0.67 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 16 | 0.67 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 19 | 0.67 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 19 | 0.67 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 19 | 0.67 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 2 | 0.67 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 8 | 0.67 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 6 | 0.67 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 10 | 0.67 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG11 | 10 | 0.67 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG12 | 10 | 0.67 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG13 | 10 | 0.67 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 7 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 19 | 0.67 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 20 | 0.67 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 3 | 0.67 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 14 | 0.67 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 12 | 0.67 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 12 | 0.67 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 12 | 0.67 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 20 | 0.67 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 20 | 0.67 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 20 | 0.67 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 12 | 0.67 |
| (1,763) | 1:103:A:SER:HB2 | 1:106:A:ASP:H | 11 | 0.67 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 3 | 0.67 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 17 | 0.67 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 17 | 0.67 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 17 | 0.67 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 10 | 0.67 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 13 | 0.67 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 13 | 0.67 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 13 | 0.67 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 13 | 0.67 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 2 | 0.67 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 4 | 0.67 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 4 | 0.67 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 4 | 0.67 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 17 | 0.67 |
| (1,441) | 1:34:A:TYR:HD2 | 1:92:A:PHE:H | 18 | 0.67 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 3 | 0.67 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 3 | 0.67 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 3 | 0.67 |
| (1,90) | 1:185:A:VAL:HA | 1:188:A:LYS:H | 5 | 0.67 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 12 | 0.67 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 12 | 0.67 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 12 | 0.67 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 12 | 0.66 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 12 | 0.66 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 11 | 0.66 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 11 | 0.66 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 13 | 0.66 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 14 | 0.66 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 14 | 0.66 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 4 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 4 | 0.66 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 20 | 0.66 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG21 | 4 | 0.66 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG22 | 4 | 0.66 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG23 | 4 | 0.66 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG21 | 4 | 0.66 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG22 | 4 | 0.66 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG23 | 4 | 0.66 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG21 | 4 | 0.66 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG22 | 4 | 0.66 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG23 | 4 | 0.66 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 4 | 0.66 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 4 | 0.66 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 4 | 0.66 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 4 | 0.66 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 4 | 0.66 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 4 | 0.66 |
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 10 | 0.66 |
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 14 | 0.66 |
| (1,2935) | 1:75:A:TRP:HA | 1:78:A:ALA:HA | 9 | 0.66 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 14 | 0.66 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 14 | 0.66 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 14 | 0.66 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 15 | 0.66 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 15 | 0.66 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 15 | 0.66 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 16 | 0.66 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 16 | 0.66 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 16 | 0.66 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 20 | 0.66 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 20 | 0.66 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 20 | 0.66 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 19 | 0.66 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 19 | 0.66 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 19 | 0.66 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 19 | 0.66 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 19 | 0.66 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 19 | 0.66 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 19 | 0.66 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 19 | 0.66 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 19 | 0.66 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 7 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 7 | 0.66 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 7 | 0.66 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 17 | 0.66 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 17 | 0.66 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 17 | 0.66 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 10 | 0.66 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 10 | 0.66 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 10 | 0.66 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 13 | 0.66 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 13 | 0.66 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 13 | 0.66 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 13 | 0.66 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 13 | 0.66 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 13 | 0.66 |
| (1,2402) | 1:174:A:VAL:HG21 | 1:175:A:ALA:HA | 18 | 0.66 |
| (1,2402) | 1:174:A:VAL:HG22 | 1:175:A:ALA:HA | 18 | 0.66 |
| (1,2402) | 1:174:A:VAL:HG23 | 1:175:A:ALA:HA | 18 | 0.66 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 14 | 0.66 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 9 | 0.66 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 9 | 0.66 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 9 | 0.66 |
| (1,2291) | 1:117:A:LYS:HG3 | 1:120:A:ASP:H | 9 | 0.66 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 17 | 0.66 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 4 | 0.66 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 4 | 0.66 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 4 | 0.66 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 4 | 0.66 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 4 | 0.66 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 4 | 0.66 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 8 | 0.66 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG11 | 3 | 0.66 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG12 | 3 | 0.66 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG13 | 3 | 0.66 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 2 | 0.66 |
| (1,1963) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HD2 | 7 | 0.66 |
| (1,1963) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HD3 | 7 | 0.66 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 17 | 0.66 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 17 | 0.66 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 17 | 0.66 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 17 | 0.66 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 17 | 0.66 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 17 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 10 | 0.66 |
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 10 | 0.66 |
| (1,1632) | 1:31:A:PRO:HA | 1:96:A:GLN:HG2 | 9 | 0.66 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 18 | 0.66 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 10 | 0.66 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 10 | 0.66 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 19 | 0.66 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 19 | 0.66 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 19 | 0.66 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 18 | 0.66 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 18 | 0.66 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 18 | 0.66 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 11 | 0.66 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 2 | 0.66 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 2 | 0.66 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 2 | 0.66 |
| (1,1298) | 1:141:A:ALA:HA | 1:146:A:LEU:HB2 | 1 | 0.66 |
| (1,1283) | 1:64:A:LEU:HA | 1:65:A:GLY:HA3 | 6 | 0.66 |
| (1,1185) | 1:29:A:TYR:HE1 | 1:68:A:GLY:H | 7 | 0.66 |
| (1,1185) | 1:29:A:TYR:HE2 | 1:68:A:GLY:H | 7 | 0.66 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 15 | 0.66 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 2 | 0.66 |
| (1,991) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HD22 | 12 | 0.66 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 10 | 0.66 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 12 | 0.66 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 17 | 0.66 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 19 | 0.66 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 7 | 0.66 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 12 | 0.66 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 19 | 0.66 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 1 | 0.66 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 1 | 0.66 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 1 | 0.66 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 3 | 0.66 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 3 | 0.66 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 3 | 0.66 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 1 | 0.66 |
| (1,416) | 1:122:A:ASP:HB3 | 1:123:A:ALA:H | 6 | 0.66 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 8 | 0.66 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 8 | 0.66 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 8 | 0.66 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 2 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 3 | 0.66 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 13 | 0.65 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 13 | 0.65 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 13 | 0.65 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 13 | 0.65 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 13 | 0.65 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 13 | 0.65 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 15 | 0.65 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 15 | 0.65 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 1 | 0.65 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD11 | 17 | 0.65 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD12 | 17 | 0.65 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD13 | 17 | 0.65 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD11 | 17 | 0.65 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD12 | 17 | 0.65 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD13 | 17 | 0.65 |
| (1,3311) | 1:29:A:TYR:HD1 | 1:71:A:LEU:HB2 | 16 | 0.65 |
| (1,3311) | 1:29:A:TYR:HD2 | 1:71:A:LEU:HB2 | 16 | 0.65 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB2 | 2 | 0.65 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB3 | 2 | 0.65 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB2 | 18 | 0.65 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB3 | 18 | 0.65 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 2 | 0.65 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 2 | 0.65 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 2 | 0.65 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 11 | 0.65 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 11 | 0.65 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 11 | 0.65 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 20 | 0.65 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 20 | 0.65 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 20 | 0.65 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 10 | 0.65 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 10 | 0.65 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 10 | 0.65 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 16 | 0.65 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 16 | 0.65 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 16 | 0.65 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 16 | 0.65 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 16 | 0.65 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 16 | 0.65 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 5 | 0.65 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 5 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 5 | 0.65 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 6 | 0.65 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 6 | 0.65 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 6 | 0.65 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 5 | 0.65 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 5 | 0.65 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 5 | 0.65 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 8 | 0.65 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 8 | 0.65 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 8 | 0.65 |
| (1,2456) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HA | 1 | 0.65 |
| (1,2456) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HA | 1 | 0.65 |
| (1,2456) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HA | 1 | 0.65 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE1 | 3 | 0.65 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE2 | 3 | 0.65 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE1 | 3 | 0.65 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE2 | 3 | 0.65 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE1 | 3 | 0.65 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE2 | 3 | 0.65 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 16 | 0.65 |
| (1,2122) | 1:10:A:ILE:HG12 | 1:159:A:GLN:HB2 | 4 | 0.65 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 4 | 0.65 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 7 | 0.65 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 7 | 0.65 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 7 | 0.65 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 7 | 0.65 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 7 | 0.65 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 7 | 0.65 |
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 20 | 0.65 |
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 20 | 0.65 |
| (1,1759) | 1:14:A:LYS:HB2 | 1:15:A:PRO:HA | 11 | 0.65 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG12 | 5 | 0.65 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG13 | 5 | 0.65 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 15 | 0.65 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 10 | 0.65 |
| (1,1669) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HG2 | 1 | 0.65 |
| (1,1669) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HG2 | 1 | 0.65 |
| (1,1669) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HG2 | 1 | 0.65 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 14 | 0.65 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 6 | 0.65 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 6 | 0.65 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 8 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 18 | 0.65 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 18 | 0.65 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 18 | 0.65 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 3 | 0.65 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 3 | 0.65 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 3 | 0.65 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG21 | 9 | 0.65 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG22 | 9 | 0.65 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG23 | 9 | 0.65 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG21 | 9 | 0.65 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG22 | 9 | 0.65 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG23 | 9 | 0.65 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG11 | 18 | 0.65 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG12 | 18 | 0.65 |
| (1,1304) | 1:40:A:LEU:HB3 | 1:42:A:VAL:HG13 | 18 | 0.65 |
| (1,1298) | 1:141:A:ALA:HA | 1:146:A:LEU:HB2 | 11 | 0.65 |
| (1,1298) | 1:141:A:ALA:HA | 1:146:A:LEU:HB2 | 14 | 0.65 |
| (1,1298) | 1:141:A:ALA:HA | 1:146:A:LEU:HB2 | 18 | 0.65 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 14 | 0.65 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 14 | 0.65 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 14 | 0.65 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 15 | 0.65 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 15 | 0.65 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 15 | 0.65 |
| (1,1137) | 1:126:A:ASN:H | 1:126:A:ASN:HB3 | 2 | 0.65 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 3 | 0.65 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 13 | 0.65 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG21 | 7 | 0.65 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG22 | 7 | 0.65 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG23 | 7 | 0.65 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 8 | 0.65 |
| (1,894) | 1:103:A:SER:H | 1:106:A:ASP:HB3 | 6 | 0.65 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 14 | 0.65 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 14 | 0.65 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 14 | 0.65 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 14 | 0.65 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 17 | 0.65 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 6 | 0.65 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 8 | 0.65 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 8 | 0.65 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 8 | 0.65 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 7 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 20 | 0.64 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 4 | 0.64 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 4 | 0.64 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 8 | 0.64 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 8 | 0.64 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 16 | 0.64 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 6 | 0.64 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 6 | 0.64 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 10 | 0.64 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 10 | 0.64 |
| (1,3311) | 1:29:A:TYR:HD1 | 1:71:A:LEU:HB2 | 4 | 0.64 |
| (1,3311) | 1:29:A:TYR:HD2 | 1:71:A:LEU:HB2 | 4 | 0.64 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 11 | 0.64 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 11 | 0.64 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 11 | 0.64 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 11 | 0.64 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 11 | 0.64 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 11 | 0.64 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 8 | 0.64 |
| (1,3269) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA2 | 6 | 0.64 |
| (1,3269) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA2 | 6 | 0.64 |
| (1,3269) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA2 | 6 | 0.64 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 1 | 0.64 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 1 | 0.64 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 1 | 0.64 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 7 | 0.64 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 7 | 0.64 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 7 | 0.64 |
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 8 | 0.64 |
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 15 | 0.64 |
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 20 | 0.64 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 11 | 0.64 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 11 | 0.64 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 11 | 0.64 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 13 | 0.64 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 13 | 0.64 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 13 | 0.64 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 20 | 0.64 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 20 | 0.64 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 20 | 0.64 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 6 | 0.64 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 6 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 6 | 0.64 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 12 | 0.64 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 12 | 0.64 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 12 | 0.64 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 13 | 0.64 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 13 | 0.64 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 13 | 0.64 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 19 | 0.64 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 19 | 0.64 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 19 | 0.64 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG21 | 16 | 0.64 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG22 | 16 | 0.64 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG23 | 16 | 0.64 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG21 | 16 | 0.64 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG22 | 16 | 0.64 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG23 | 16 | 0.64 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 16 | 0.64 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 16 | 0.64 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 16 | 0.64 |
| (1,2602) | 1:47:A:ARG:HG2 | 1:48:A:GLN:HA | 10 | 0.64 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 20 | 0.64 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 20 | 0.64 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 20 | 0.64 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 10 | 0.64 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 10 | 0.64 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 10 | 0.64 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 12 | 0.64 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 12 | 0.64 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 12 | 0.64 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 9 | 0.64 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 9 | 0.64 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 9 | 0.64 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 9 | 0.64 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 9 | 0.64 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 9 | 0.64 |
| (1,2452) | 1:149:A:VAL:HG11 | 1:150:A:PRO:HG3 | 7 | 0.64 |
| (1,2452) | 1:149:A:VAL:HG12 | 1:150:A:PRO:HG3 | 7 | 0.64 |
| (1,2452) | 1:149:A:VAL:HG13 | 1:150:A:PRO:HG3 | 7 | 0.64 |
| (1,2452) | 1:149:A:VAL:HG21 | 1:150:A:PRO:HG3 | 7 | 0.64 |
| (1,2452) | 1:149:A:VAL:HG22 | 1:150:A:PRO:HG3 | 7 | 0.64 |
| (1,2452) | 1:149:A:VAL:HG23 | 1:150:A:PRO:HG3 | 7 | 0.64 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 8 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 3 | 0.64 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 11 | 0.64 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 11 | 0.64 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 11 | 0.64 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 11 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG11 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG12 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG13 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG21 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG22 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG23 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG11 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG12 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG13 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG21 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG22 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG23 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG11 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG12 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG13 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG21 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG22 | 3 | 0.64 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG23 | 3 | 0.64 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 5 | 0.64 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 5 | 0.64 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 5 | 0.64 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 5 | 0.64 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 5 | 0.64 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 5 | 0.64 |
| (1,2168) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HG2 | 17 | 0.64 |
| (1,2168) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HG2 | 17 | 0.64 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 14 | 0.64 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD1 | 10 | 0.64 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD2 | 10 | 0.64 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 14 | 0.64 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 12 | 0.64 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 12 | 0.64 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 12 | 0.64 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG21 | 15 | 0.64 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG22 | 15 | 0.64 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG23 | 15 | 0.64 |
| (1,1813) | 1:160:A:LEU:HD21 | 1:180:A:THR:HB | 4 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1813) | 1:160:A:LEU:HD22 | 1:180:A:THR:HB | 4 | 0.64 |
| (1,1813) | 1:160:A:LEU:HD23 | 1:180:A:THR:HB | 4 | 0.64 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 3 | 0.64 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 5 | 0.64 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 5 | 0.64 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 5 | 0.64 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 14 | 0.64 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 4 | 0.64 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 4 | 0.64 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 19 | 0.64 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 1 | 0.64 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 1 | 0.64 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 1 | 0.64 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 19 | 0.64 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 19 | 0.64 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 19 | 0.64 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 3 | 0.64 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 12 | 0.64 |
| (1,1358) | 1:179:A:ASP:HB3 | 1:183:A:GLN:HE21 | 9 | 0.64 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 17 | 0.64 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 17 | 0.64 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 17 | 0.64 |
| (1,1262) | 1:29:A:TYR:HB3 | 1:64:A:LEU:HB2 | 19 | 0.64 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 14 | 0.64 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 11 | 0.64 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 11 | 0.64 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 11 | 0.64 |
| (1,1080) | 1:34:A:TYR:HD2 | 1:38:A:GLU:H | 9 | 0.64 |
| (1,1058) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HA | 10 | 0.64 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 5 | 0.64 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 8 | 0.64 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 20 | 0.64 |
| (1,894) | 1:103:A:SER:H | 1:106:A:ASP:HB3 | 1 | 0.64 |
| (1,894) | 1:103:A:SER:H | 1:106:A:ASP:HB3 | 9 | 0.64 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 8 | 0.64 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 15 | 0.64 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 10 | 0.64 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 10 | 0.64 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 10 | 0.64 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 9 | 0.64 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 14 | 0.64 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 12 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,441) | 1:34:A:TYR:HE2 | 1:92:A:PHE:H | 4 | 0.64 |
| (1,416) | 1:122:A:ASP:HB3 | 1:123:A:ALA:H | 14 | 0.64 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 16 | 0.64 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 4 | 0.64 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 4 | 0.64 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 4 | 0.64 |
| (1,266) | 1:67:A:LEU:HD11 | 1:70:A:ASP:H | 11 | 0.64 |
| (1,266) | 1:67:A:LEU:HD12 | 1:70:A:ASP:H | 11 | 0.64 |
| (1,266) | 1:67:A:LEU:HD13 | 1:70:A:ASP:H | 11 | 0.64 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 17 | 0.64 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 17 | 0.64 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 17 | 0.64 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 4 | 0.64 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 4 | 0.64 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 7 | 0.64 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 7 | 0.64 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 7 | 0.64 |
| (1,128) | 1:12:A:LEU:HD11 | 1:159:A:GLN:H | 15 | 0.64 |
| (1,128) | 1:12:A:LEU:HD12 | 1:159:A:GLN:H | 15 | 0.64 |
| (1,128) | 1:12:A:LEU:HD13 | 1:159:A:GLN:H | 15 | 0.64 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 3 | 0.63 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 3 | 0.63 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 1 | 0.63 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 11 | 0.63 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 15 | 0.63 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 15 | 0.63 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD11 | 12 | 0.63 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD12 | 12 | 0.63 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD13 | 12 | 0.63 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD11 | 12 | 0.63 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD12 | 12 | 0.63 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD13 | 12 | 0.63 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 4 | 0.63 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 17 | 0.63 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 20 | 0.63 |
| (1,3274) | 1:118:A:GLY:HA3 | 1:121:A:TYR:H | 14 | 0.63 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 17 | 0.63 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 17 | 0.63 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 17 | 0.63 |
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 5 | 0.63 |
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 6 | 0.63 |
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 16 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 20 | 0.63 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 14 | 0.63 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 14 | 0.63 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 14 | 0.63 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 8 | 0.63 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 8 | 0.63 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 8 | 0.63 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 17 | 0.63 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 17 | 0.63 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 17 | 0.63 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG21 | 3 | 0.63 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG22 | 3 | 0.63 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG23 | 3 | 0.63 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG21 | 3 | 0.63 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG22 | 3 | 0.63 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG23 | 3 | 0.63 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG21 | 10 | 0.63 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG22 | 10 | 0.63 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG23 | 10 | 0.63 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG21 | 10 | 0.63 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG22 | 10 | 0.63 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG23 | 10 | 0.63 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 11 | 0.63 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 11 | 0.63 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 11 | 0.63 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 1 | 0.63 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 1 | 0.63 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 1 | 0.63 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 4 | 0.63 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 4 | 0.63 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 4 | 0.63 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 4 | 0.63 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 4 | 0.63 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 4 | 0.63 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 4 | 0.63 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 4 | 0.63 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 4 | 0.63 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 17 | 0.63 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 17 | 0.63 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 17 | 0.63 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 13 | 0.63 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 4 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 4 | 0.63 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 4 | 0.63 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 18 | 0.63 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 18 | 0.63 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 18 | 0.63 |
| (1,2456) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HA | 11 | 0.63 |
| (1,2456) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HA | 11 | 0.63 |
| (1,2456) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HA | 11 | 0.63 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 1 | 0.63 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 1 | 0.63 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 1 | 0.63 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 2 | 0.63 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 2 | 0.63 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 2 | 0.63 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 8 | 0.63 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 8 | 0.63 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 8 | 0.63 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 10 | 0.63 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 10 | 0.63 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 10 | 0.63 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 18 | 0.63 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 18 | 0.63 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 18 | 0.63 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 1 | 0.63 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 14 | 0.63 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 17 | 0.63 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 20 | 0.63 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 20 | 0.63 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 20 | 0.63 |
| (1,2316) | 1:117:A:LYS:H | 1:117:A:LYS:HG2 | 8 | 0.63 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 17 | 0.63 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 17 | 0.63 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 17 | 0.63 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 17 | 0.63 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 17 | 0.63 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 17 | 0.63 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 3 | 0.63 |
| (1,2014) | 1:117:A:LYS:HA | 1:117:A:LYS:HD3 | 15 | 0.63 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 14 | 0.63 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 14 | 0.63 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 14 | 0.63 |
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 7 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 7 | 0.63 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 11 | 0.63 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 13 | 0.63 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 13 | 0.63 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 13 | 0.63 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 16 | 0.63 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 16 | 0.63 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 10 | 0.63 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 10 | 0.63 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 10 | 0.63 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 15 | 0.63 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE2 | 16 | 0.63 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE3 | 16 | 0.63 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE2 | 16 | 0.63 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE3 | 16 | 0.63 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE2 | 16 | 0.63 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE3 | 16 | 0.63 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 8 | 0.63 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 20 | 0.63 |
| (1,1213) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE21 | 14 | 0.63 |
| (1,1213) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE21 | 14 | 0.63 |
| (1,1213) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE21 | 14 | 0.63 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 2 | 0.63 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 2 | 0.63 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 2 | 0.63 |
| (1,1137) | 1:126:A:ASN:H | 1:126:A:ASN:HB3 | 9 | 0.63 |
| (1,1084) | 1:37:A:GLU:HG3 | 1:38:A:GLU:H | 19 | 0.63 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 2 | 0.63 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 9 | 0.63 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 17 | 0.63 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 20 | 0.63 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 15 | 0.63 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 15 | 0.63 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 15 | 0.63 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 20 | 0.63 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 20 | 0.63 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 20 | 0.63 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 9 | 0.63 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 9 | 0.63 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 9 | 0.63 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 4 | 0.63 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 17 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 17 | 0.63 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 17 | 0.63 |
| (1,492) | 1:138:A:GLU:HB2 | 1:140:A:ALA:H | 15 | 0.63 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 16 | 0.63 |
| (1,441) | 1:34:A:TYR:HE2 | 1:92:A:PHE:H | 5 | 0.63 |
| (1,441) | 1:34:A:TYR:HE1 | 1:92:A:PHE:H | 9 | 0.63 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 4 | 0.62 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 4 | 0.62 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 9 | 0.62 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 9 | 0.62 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 14 | 0.62 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 14 | 0.62 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 14 | 0.62 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 14 | 0.62 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 15 | 0.62 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 15 | 0.62 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 15 | 0.62 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 15 | 0.62 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 15 | 0.62 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 15 | 0.62 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 3 | 0.62 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 3 | 0.62 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 16 | 0.62 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 16 | 0.62 |
| (1,3297) | 1:23:A:LEU:HB2 | 1:153:A:TYR:H | 15 | 0.62 |
| (1,3296) | 1:16:A:ILE:HG21 | 1:156:A:GLY:HA3 | 6 | 0.62 |
| (1,3296) | 1:16:A:ILE:HG22 | 1:156:A:GLY:HA3 | 6 | 0.62 |
| (1,3296) | 1:16:A:ILE:HG23 | 1:156:A:GLY:HA3 | 6 | 0.62 |
| (1,3274) | 1:118:A:GLY:HA3 | 1:121:A:TYR:H | 11 | 0.62 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE1 | 14 | 0.62 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE2 | 14 | 0.62 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE3 | 14 | 0.62 |
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 4 | 0.62 |
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 14 | 0.62 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 16 | 0.62 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 16 | 0.62 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 16 | 0.62 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 7 | 0.62 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 7 | 0.62 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 7 | 0.62 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 12 | 0.62 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 12 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 12 | 0.62 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 8 | 0.62 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 8 | 0.62 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 8 | 0.62 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 8 | 0.62 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 8 | 0.62 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 8 | 0.62 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 8 | 0.62 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 8 | 0.62 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 8 | 0.62 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 4 | 0.62 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 4 | 0.62 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 4 | 0.62 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 11 | 0.62 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 11 | 0.62 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 11 | 0.62 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 14 | 0.62 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 14 | 0.62 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 14 | 0.62 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 15 | 0.62 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 15 | 0.62 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 15 | 0.62 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 20 | 0.62 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 20 | 0.62 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 20 | 0.62 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 12 | 0.62 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 12 | 0.62 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 12 | 0.62 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 8 | 0.62 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 8 | 0.62 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 8 | 0.62 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 3 | 0.62 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 3 | 0.62 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 3 | 0.62 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 14 | 0.62 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 14 | 0.62 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 14 | 0.62 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 15 | 0.62 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 15 | 0.62 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 15 | 0.62 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 16 | 0.62 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 16 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 16 | 0.62 |
| (1,2316) | 1:117:A:LYS:H | 1:117:A:LYS:HG2 | 9 | 0.62 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 10 | 0.62 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 10 | 0.62 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 10 | 0.62 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 19 | 0.62 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 19 | 0.62 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 19 | 0.62 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 11 | 0.62 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD11 | 3 | 0.62 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD12 | 3 | 0.62 |
| (1,1983) | 1:66:A:PRO:HA | 1:67:A:LEU:HD13 | 3 | 0.62 |
| (1,1813) | 1:160:A:LEU:HD21 | 1:180:A:THR:HB | 13 | 0.62 |
| (1,1813) | 1:160:A:LEU:HD22 | 1:180:A:THR:HB | 13 | 0.62 |
| (1,1813) | 1:160:A:LEU:HD23 | 1:180:A:THR:HB | 13 | 0.62 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD1 | 18 | 0.62 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD2 | 18 | 0.62 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 18 | 0.62 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 18 | 0.62 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 18 | 0.62 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 9 | 0.62 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 9 | 0.62 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 9 | 0.62 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 9 | 0.62 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 9 | 0.62 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 9 | 0.62 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 20 | 0.62 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 20 | 0.62 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 20 | 0.62 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 5 | 0.62 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 5 | 0.62 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 17 | 0.62 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 17 | 0.62 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 12 | 0.62 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 12 | 0.62 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 12 | 0.62 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 12 | 0.62 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 13 | 0.62 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 13 | 0.62 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 13 | 0.62 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 6 | 0.62 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 6 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 6 | 0.62 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 13 | 0.62 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 13 | 0.62 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 13 | 0.62 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 17 | 0.62 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 17 | 0.62 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 17 | 0.62 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 7 | 0.62 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE2 | 14 | 0.62 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE3 | 14 | 0.62 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE2 | 14 | 0.62 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE3 | 14 | 0.62 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE2 | 14 | 0.62 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE3 | 14 | 0.62 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE2 | 18 | 0.62 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE3 | 18 | 0.62 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE2 | 18 | 0.62 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE3 | 18 | 0.62 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE2 | 18 | 0.62 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE3 | 18 | 0.62 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 5 | 0.62 |
| (1,1298) | 1:141:A:ALA:HA | 1:146:A:LEU:HB2 | 19 | 0.62 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 12 | 0.62 |
| (1,1191) | 1:64:A:LEU:HD11 | 1:65:A:GLY:H | 19 | 0.62 |
| (1,1191) | 1:64:A:LEU:HD12 | 1:65:A:GLY:H | 19 | 0.62 |
| (1,1191) | 1:64:A:LEU:HD13 | 1:65:A:GLY:H | 19 | 0.62 |
| (1,1137) | 1:126:A:ASN:H | 1:126:A:ASN:HB3 | 6 | 0.62 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 4 | 0.62 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 6 | 0.62 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 10 | 0.62 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 12 | 0.62 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 9 | 0.62 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 4 | 0.62 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 4 | 0.62 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 4 | 0.62 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 4 | 0.62 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 13 | 0.62 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 13 | 0.62 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 13 | 0.62 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 3 | 0.62 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 5 | 0.62 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 20 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 9 | 0.62 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 13 | 0.62 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 3 | 0.62 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 6 | 0.62 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 8 | 0.62 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 8 | 0.62 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 8 | 0.62 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 14 | 0.62 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 14 | 0.62 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 14 | 0.62 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 16 | 0.62 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 16 | 0.62 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 16 | 0.62 |
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 19 | 0.62 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 9 | 0.61 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 9 | 0.61 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 9 | 0.61 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 9 | 0.61 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 9 | 0.61 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 9 | 0.61 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 20 | 0.61 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG11 | 18 | 0.61 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG12 | 18 | 0.61 |
| (1,3370) | 1:173:A:PHE:HD1 | 1:174:A:VAL:HG13 | 18 | 0.61 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG11 | 18 | 0.61 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG12 | 18 | 0.61 |
| (1,3370) | 1:173:A:PHE:HD2 | 1:174:A:VAL:HG13 | 18 | 0.61 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 17 | 0.61 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 17 | 0.61 |
| (1,3297) | 1:23:A:LEU:HB2 | 1:153:A:TYR:H | 2 | 0.61 |
| (1,3269) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA2 | 10 | 0.61 |
| (1,3269) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA2 | 10 | 0.61 |
| (1,3269) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA2 | 10 | 0.61 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 19 | 0.61 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 19 | 0.61 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 19 | 0.61 |
| (1,3076) | 1:47:A:ARG:HG3 | 1:56:A:MET:HE1 | 11 | 0.61 |
| (1,3076) | 1:47:A:ARG:HG3 | 1:56:A:MET:HE2 | 11 | 0.61 |
| (1,3076) | 1:47:A:ARG:HG3 | 1:56:A:MET:HE3 | 11 | 0.61 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE1 | 16 | 0.61 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE2 | 16 | 0.61 |
| (1,3075) | 1:56:A:MET:HG3 | 1:56:A:MET:HE3 | 16 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 13 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 13 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 13 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 13 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 13 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 13 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 13 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 13 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 13 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 13 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 20 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 20 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 20 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 20 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 20 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 20 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 20 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 20 | 0.61 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 20 | 0.61 |
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 2 | 0.61 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 2 | 0.61 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 2 | 0.61 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 1 | 0.61 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 1 | 0.61 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 1 | 0.61 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 15 | 0.61 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 15 | 0.61 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 15 | 0.61 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 15 | 0.61 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 15 | 0.61 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 15 | 0.61 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 15 | 0.61 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 15 | 0.61 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 15 | 0.61 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 3 | 0.61 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 3 | 0.61 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 3 | 0.61 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 3 | 0.61 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 3 | 0.61 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 3 | 0.61 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 2 | 0.61 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 2 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 2 | 0.61 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 7 | 0.61 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 7 | 0.61 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 7 | 0.61 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 3 | 0.61 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 3 | 0.61 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 3 | 0.61 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 3 | 0.61 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 3 | 0.61 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 3 | 0.61 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 3 | 0.61 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 3 | 0.61 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 3 | 0.61 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 20 | 0.61 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 20 | 0.61 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 20 | 0.61 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 3 | 0.61 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 3 | 0.61 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 3 | 0.61 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 12 | 0.61 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 12 | 0.61 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 12 | 0.61 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 15 | 0.61 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 15 | 0.61 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 15 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 4 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 4 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 4 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 5 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 5 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 5 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 6 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 6 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 6 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 9 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 9 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 9 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 11 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 11 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 11 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 12 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 12 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 12 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 13 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 13 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 13 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 20 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 20 | 0.61 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 20 | 0.61 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 16 | 0.61 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 19 | 0.61 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 4 | 0.61 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 19 | 0.61 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 19 | 0.61 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 19 | 0.61 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 19 | 0.61 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 19 | 0.61 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 19 | 0.61 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 3 | 0.61 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 3 | 0.61 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 3 | 0.61 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 3 | 0.61 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 3 | 0.61 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 3 | 0.61 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 3 | 0.61 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 3 | 0.61 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 3 | 0.61 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 2 | 0.61 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 2 | 0.61 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 2 | 0.61 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 2 | 0.61 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 2 | 0.61 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 2 | 0.61 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 2 | 0.61 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 15 | 0.61 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 5 | 0.61 |
| (1,1652) | 1:38:A:GLU:HG2 | 1:41:A:HIS:HE1 | 14 | 0.61 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 9 | 0.61 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 9 | 0.61 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 9 | 0.61 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 3 | 0.61 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 3 | 0.61 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 3 | 0.61 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 20 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 20 | 0.61 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 1 | 0.61 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 1 | 0.61 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 1 | 0.61 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 12 | 0.61 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 12 | 0.61 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 12 | 0.61 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 18 | 0.61 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 18 | 0.61 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 18 | 0.61 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 16 | 0.61 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 16 | 0.61 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 16 | 0.61 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 19 | 0.61 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 19 | 0.61 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 19 | 0.61 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 6 | 0.61 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE2 | 11 | 0.61 |
| (1,1355) | 1:15:A:PRO:HD2 | 1:157:A:LYS:HE3 | 11 | 0.61 |
| (1,1283) | 1:64:A:LEU:HA | 1:65:A:GLY:HA3 | 20 | 0.61 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 3 | 0.61 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 4 | 0.61 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 17 | 0.61 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 17 | 0.61 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 17 | 0.61 |
| (1,1084) | 1:37:A:GLU:HG3 | 1:38:A:GLU:H | 3 | 0.61 |
| (1,1084) | 1:37:A:GLU:HG3 | 1:38:A:GLU:H | 17 | 0.61 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 8 | 0.61 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 11 | 0.61 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 14 | 0.61 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 5 | 0.61 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 6 | 0.61 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 9 | 0.61 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 19 | 0.61 |
| (1,894) | 1:103:A:SER:H | 1:106:A:ASP:HB3 | 16 | 0.61 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 18 | 0.61 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 2 | 0.61 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 2 | 0.61 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 2 | 0.61 |
| (1,799) | 1:49:A:LYS:HG2 | 1:179:A:ASP:H | 13 | 0.61 |
| (1,799) | 1:49:A:LYS:HG3 | 1:179:A:ASP:H | 13 | 0.61 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 8 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 12 | 0.61 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 12 | 0.61 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 12 | 0.61 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 19 | 0.61 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 19 | 0.61 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 19 | 0.61 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 9 | 0.61 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 11 | 0.61 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 2 | 0.61 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 10 | 0.61 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 5 | 0.61 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 5 | 0.61 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 5 | 0.61 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 12 | 0.61 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 12 | 0.61 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 12 | 0.61 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 13 | 0.61 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 13 | 0.61 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 13 | 0.61 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 5 | 0.61 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 5 | 0.61 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 5 | 0.61 |
| (1,242) | 1:145:A:GLN:HE21 | 1:147:A:GLN:H | 14 | 0.61 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 6 | 0.6 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 6 | 0.6 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 6 | 0.6 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 6 | 0.6 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 6 | 0.6 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 6 | 0.6 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 3 | 0.6 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 3 | 0.6 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 17 | 0.6 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 7 | 0.6 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 7 | 0.6 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 11 | 0.6 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 11 | 0.6 |
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 5 | 0.6 |
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 5 | 0.6 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD1 | 20 | 0.6 |
| (1,3372) | 1:42:A:VAL:HG11 | 1:173:A:PHE:HD2 | 20 | 0.6 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD1 | 20 | 0.6 |
| (1,3372) | 1:42:A:VAL:HG12 | 1:173:A:PHE:HD2 | 20 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD1 | 20 | 0.6 |
| (1,3372) | 1:42:A:VAL:HG13 | 1:173:A:PHE:HD2 | 20 | 0.6 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 7 | 0.6 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 7 | 0.6 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 16 | 0.6 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 16 | 0.6 |
| (1,3297) | 1:23:A:LEU:HB2 | 1:153:A:TYR:H | 12 | 0.6 |
| (1,3269) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA2 | 4 | 0.6 |
| (1,3269) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA2 | 4 | 0.6 |
| (1,3269) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA2 | 4 | 0.6 |
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 3 | 0.6 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 2 | 0.6 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 2 | 0.6 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 2 | 0.6 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 16 | 0.6 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 16 | 0.6 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 16 | 0.6 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 18 | 0.6 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 14 | 0.6 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 14 | 0.6 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 14 | 0.6 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 14 | 0.6 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 14 | 0.6 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 14 | 0.6 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 14 | 0.6 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 14 | 0.6 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 14 | 0.6 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 1 | 0.6 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 1 | 0.6 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 1 | 0.6 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 6 | 0.6 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 6 | 0.6 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 6 | 0.6 |
| (1,2668) | 1:45:A:ASN:HA | 1:48:A:GLN:HB3 | 18 | 0.6 |
| (1,2452) | 1:149:A:VAL:HG11 | 1:150:A:PRO:HG3 | 20 | 0.6 |
| (1,2452) | 1:149:A:VAL:HG12 | 1:150:A:PRO:HG3 | 20 | 0.6 |
| (1,2452) | 1:149:A:VAL:HG13 | 1:150:A:PRO:HG3 | 20 | 0.6 |
| (1,2452) | 1:149:A:VAL:HG21 | 1:150:A:PRO:HG3 | 20 | 0.6 |
| (1,2452) | 1:149:A:VAL:HG22 | 1:150:A:PRO:HG3 | 20 | 0.6 |
| (1,2452) | 1:149:A:VAL:HG23 | 1:150:A:PRO:HG3 | 20 | 0.6 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 17 | 0.6 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 17 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 17 | 0.6 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 18 | 0.6 |
| (1,2316) | 1:117:A:LYS:H | 1:117:A:LYS:HG2 | 17 | 0.6 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 15 | 0.6 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 15 | 0.6 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 15 | 0.6 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 14 | 0.6 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 14 | 0.6 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 14 | 0.6 |
| (1,2171) | 1:86:A:LYS:H | 1:87:A:ILE:HG12 | 16 | 0.6 |
| (1,2171) | 1:86:A:LYS:H | 1:87:A:ILE:HG12 | 20 | 0.6 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 14 | 0.6 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 14 | 0.6 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 14 | 0.6 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 14 | 0.6 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 14 | 0.6 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 14 | 0.6 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 8 | 0.6 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 8 | 0.6 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 8 | 0.6 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG11 | 9 | 0.6 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG12 | 9 | 0.6 |
| (1,1966) | 1:38:A:GLU:HB3 | 1:39:A:VAL:HG13 | 9 | 0.6 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG21 | 18 | 0.6 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG22 | 18 | 0.6 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG23 | 18 | 0.6 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 4 | 0.6 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 4 | 0.6 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 4 | 0.6 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 4 | 0.6 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 4 | 0.6 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 4 | 0.6 |
| (1,1813) | 1:160:A:LEU:HD21 | 1:180:A:THR:HB | 10 | 0.6 |
| (1,1813) | 1:160:A:LEU:HD22 | 1:180:A:THR:HB | 10 | 0.6 |
| (1,1813) | 1:160:A:LEU:HD23 | 1:180:A:THR:HB | 10 | 0.6 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 10 | 0.6 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 10 | 0.6 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 10 | 0.6 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 10 | 0.6 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 10 | 0.6 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 10 | 0.6 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 12 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 12 | 0.6 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 12 | 0.6 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 12 | 0.6 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 12 | 0.6 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 12 | 0.6 |
| (1,1686) | 1:99:A:GLN:HG3 | 1:100:A:THR:H | 11 | 0.6 |
| (1,1686) | 1:99:A:GLN:HG3 | 1:100:A:THR:H | 18 | 0.6 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE1 | 3 | 0.6 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE2 | 3 | 0.6 |
| (1,1559) | 1:156:A:GLY:HA2 | 1:157:A:LYS:HB2 | 2 | 0.6 |
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 11 | 0.6 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 11 | 0.6 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 11 | 0.6 |
| (1,1409) | 1:67:A:LEU:HB2 | 1:70:A:ASP:HB3 | 1 | 0.6 |
| (1,1366) | 1:34:A:TYR:HE1 | 1:97:A:LYS:HE3 | 7 | 0.6 |
| (1,1366) | 1:34:A:TYR:HE2 | 1:97:A:LYS:HE3 | 7 | 0.6 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE2 | 11 | 0.6 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE3 | 11 | 0.6 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE2 | 11 | 0.6 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE3 | 11 | 0.6 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE2 | 11 | 0.6 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE3 | 11 | 0.6 |
| (1,1298) | 1:141:A:ALA:HA | 1:146:A:LEU:HB2 | 6 | 0.6 |
| (1,1164) | 1:27:A:SER:H | 1:30:A:CYS:HB3 | 14 | 0.6 |
| (1,1137) | 1:126:A:ASN:H | 1:126:A:ASN:HB3 | 8 | 0.6 |
| (1,1058) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HA | 18 | 0.6 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 3 | 0.6 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 3 | 0.6 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 3 | 0.6 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 12 | 0.6 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 12 | 0.6 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 12 | 0.6 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 5 | 0.6 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 5 | 0.6 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 5 | 0.6 |
| (1,683) | 1:168:A:SER:H | 1:170:A:MET:HG2 | 15 | 0.6 |
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 12 | 0.6 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 2 | 0.6 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 2 | 0.6 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 2 | 0.6 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 3 | 0.6 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 3 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 3 | 0.6 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 6 | 0.6 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 6 | 0.6 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 6 | 0.6 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 12 | 0.6 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 12 | 0.6 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 12 | 0.6 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 4 | 0.6 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 4 | 0.6 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 4 | 0.6 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 16 | 0.6 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 16 | 0.6 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 16 | 0.6 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 18 | 0.6 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 18 | 0.6 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 18 | 0.6 |
| (1,242) | 1:145:A:GLN:HE21 | 1:147:A:GLN:H | 1 | 0.6 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 18 | 0.6 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 18 | 0.6 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 18 | 0.6 |
| (1,163) | 1:69:A:LYS:H | 1:70:A:ASP:HB3 | 3 | 0.6 |
| (1,128) | 1:12:A:LEU:HD11 | 1:159:A:GLN:H | 9 | 0.6 |
| (1,128) | 1:12:A:LEU:HD12 | 1:159:A:GLN:H | 9 | 0.6 |
| (1,128) | 1:12:A:LEU:HD13 | 1:159:A:GLN:H | 9 | 0.6 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 2 | 0.59 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 15 | 0.59 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 20 | 0.59 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 13 | 0.59 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 13 | 0.59 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 16 | 0.59 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 16 | 0.59 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB2 | 12 | 0.59 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB3 | 12 | 0.59 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG11 | 1 | 0.59 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG12 | 1 | 0.59 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG13 | 1 | 0.59 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 8 | 0.59 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 8 | 0.59 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 8 | 0.59 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 8 | 0.59 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 8 | 0.59 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 8 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 8 | 0.59 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 8 | 0.59 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 8 | 0.59 |
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 1 | 0.59 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 7 | 0.59 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 7 | 0.59 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 7 | 0.59 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 5 | 0.59 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 5 | 0.59 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 5 | 0.59 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 6 | 0.59 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 6 | 0.59 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 6 | 0.59 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 17 | 0.59 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 17 | 0.59 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 17 | 0.59 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 1 | 0.59 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 1 | 0.59 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 1 | 0.59 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG11 | 8 | 0.59 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG12 | 8 | 0.59 |
| (1,2593) | 1:37:A:GLU:HA | 1:42:A:VAL:HG13 | 8 | 0.59 |
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 17 | 0.59 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 17 | 0.59 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 17 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 1 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 1 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 1 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 1 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 1 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 1 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 1 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 1 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 1 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 16 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 16 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 16 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 16 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 16 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 16 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 16 | 0.59 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 16 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 16 | 0.59 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 19 | 0.59 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 19 | 0.59 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 19 | 0.59 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 17 | 0.59 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 17 | 0.59 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 17 | 0.59 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 19 | 0.59 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 19 | 0.59 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 19 | 0.59 |
| (1,2452) | 1:149:A:VAL:HG11 | 1:150:A:PRO:HG3 | 2 | 0.59 |
| (1,2452) | 1:149:A:VAL:HG12 | 1:150:A:PRO:HG3 | 2 | 0.59 |
| (1,2452) | 1:149:A:VAL:HG13 | 1:150:A:PRO:HG3 | 2 | 0.59 |
| (1,2452) | 1:149:A:VAL:HG21 | 1:150:A:PRO:HG3 | 2 | 0.59 |
| (1,2452) | 1:149:A:VAL:HG22 | 1:150:A:PRO:HG3 | 2 | 0.59 |
| (1,2452) | 1:149:A:VAL:HG23 | 1:150:A:PRO:HG3 | 2 | 0.59 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 6 | 0.59 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 6 | 0.59 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 6 | 0.59 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 6 | 0.59 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 17 | 0.59 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 17 | 0.59 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 17 | 0.59 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 3 | 0.59 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 14 | 0.59 |
| (1,2171) | 1:86:A:LYS:H | 1:87:A:ILE:HG12 | 4 | 0.59 |
| (1,2165) | 1:8:A:GLN:HB3 | 1:9:A:TYR:HD1 | 19 | 0.59 |
| (1,2165) | 1:8:A:GLN:HB3 | 1:9:A:TYR:HD2 | 19 | 0.59 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 7 | 0.59 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 7 | 0.59 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 7 | 0.59 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 15 | 0.59 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 15 | 0.59 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 15 | 0.59 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 5 | 0.59 |
| (1,1931) | 1:62:A:GLU:HB2 | 1:63:A:PHE:HB3 | 6 | 0.59 |
| (1,1931) | 1:62:A:GLU:HB3 | 1:63:A:PHE:HB3 | 6 | 0.59 |
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 14 | 0.59 |
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 14 | 0.59 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 6 | 0.59 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 6 | 0.59 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 6 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 6 | 0.59 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 6 | 0.59 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 6 | 0.59 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 11 | 0.59 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 11 | 0.59 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 11 | 0.59 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 11 | 0.59 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 11 | 0.59 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 11 | 0.59 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 6 | 0.59 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 17 | 0.59 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 10 | 0.59 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 10 | 0.59 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 10 | 0.59 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 13 | 0.59 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 13 | 0.59 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 13 | 0.59 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 14 | 0.59 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 14 | 0.59 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 14 | 0.59 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 18 | 0.59 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 18 | 0.59 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 18 | 0.59 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 15 | 0.59 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 15 | 0.59 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 15 | 0.59 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 7 | 0.59 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 7 | 0.59 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 7 | 0.59 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 16 | 0.59 |
| (1,1358) | 1:179:A:ASP:HB3 | 1:183:A:GLN:HE21 | 12 | 0.59 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE2 | 10 | 0.59 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE3 | 10 | 0.59 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE2 | 10 | 0.59 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE3 | 10 | 0.59 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE2 | 10 | 0.59 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE3 | 10 | 0.59 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 12 | 0.59 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 8 | 0.59 |
| (1,1191) | 1:64:A:LEU:HD11 | 1:65:A:GLY:H | 13 | 0.59 |
| (1,1191) | 1:64:A:LEU:HD12 | 1:65:A:GLY:H | 13 | 0.59 |
| (1,1191) | 1:64:A:LEU:HD13 | 1:65:A:GLY:H | 13 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 6 | 0.59 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 6 | 0.59 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 6 | 0.59 |
| (1,1080) | 1:34:A:TYR:HD1 | 1:38:A:GLU:H | 8 | 0.59 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 14 | 0.59 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 2 | 0.59 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 12 | 0.59 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 20 | 0.59 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 19 | 0.59 |
| (1,894) | 1:103:A:SER:H | 1:106:A:ASP:HB3 | 14 | 0.59 |
| (1,883) | 1:49:A:LYS:H | 1:49:A:LYS:HD3 | 14 | 0.59 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD21 | 14 | 0.59 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD22 | 14 | 0.59 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD23 | 14 | 0.59 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 13 | 0.59 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 13 | 0.59 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 13 | 0.59 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 2 | 0.59 |
| (1,765) | 1:106:A:ASP:H | 1:106:A:ASP:HB3 | 2 | 0.59 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 18 | 0.59 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 11 | 0.59 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 11 | 0.59 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 11 | 0.59 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 11 | 0.59 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 11 | 0.59 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 11 | 0.59 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 2 | 0.59 |
| (1,441) | 1:34:A:TYR:HE1 | 1:92:A:PHE:H | 10 | 0.59 |
| (1,441) | 1:34:A:TYR:HE2 | 1:92:A:PHE:H | 17 | 0.59 |
| (1,441) | 1:34:A:TYR:HD2 | 1:92:A:PHE:H | 19 | 0.59 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 14 | 0.59 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 14 | 0.59 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 14 | 0.59 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 15 | 0.59 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 15 | 0.59 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 15 | 0.59 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 20 | 0.59 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 20 | 0.59 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 20 | 0.59 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 12 | 0.59 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 12 | 0.59 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 12 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 18 | 0.59 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 18 | 0.59 |
| (1,127) | 1:105:A:ALA:H | 1:107:A:ILE:HB | 2 | 0.59 |
| (1,127) | 1:105:A:ALA:H | 1:107:A:ILE:HB | 6 | 0.59 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG11 | 18 | 0.59 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG12 | 18 | 0.59 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG13 | 18 | 0.59 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 10 | 0.59 |
| (1,78) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 4 | 0.59 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 12 | 0.58 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 12 | 0.58 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 1 | 0.58 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 4 | 0.58 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 6 | 0.58 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 9 | 0.58 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 11 | 0.58 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 19 | 0.58 |
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 9 | 0.58 |
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 9 | 0.58 |
| (1,3415) | 1:59:A:TYR:HD1 | 1:137:A:GLN:HG3 | 17 | 0.58 |
| (1,3415) | 1:59:A:TYR:HD2 | 1:137:A:GLN:HG3 | 17 | 0.58 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD11 | 4 | 0.58 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD12 | 4 | 0.58 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD13 | 4 | 0.58 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD11 | 4 | 0.58 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD12 | 4 | 0.58 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD13 | 4 | 0.58 |
| (1,3277) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA3 | 6 | 0.58 |
| (1,3277) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA3 | 6 | 0.58 |
| (1,3277) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA3 | 6 | 0.58 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 18 | 0.58 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 18 | 0.58 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 18 | 0.58 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 18 | 0.58 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 18 | 0.58 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 18 | 0.58 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD21 | 1 | 0.58 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD22 | 1 | 0.58 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD23 | 1 | 0.58 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD21 | 1 | 0.58 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD22 | 1 | 0.58 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD23 | 1 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD21 | 1 | 0.58 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD22 | 1 | 0.58 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD23 | 1 | 0.58 |
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 12 | 0.58 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 12 | 0.58 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 12 | 0.58 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 7 | 0.58 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 7 | 0.58 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 7 | 0.58 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 2 | 0.58 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 2 | 0.58 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 2 | 0.58 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG21 | 13 | 0.58 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG22 | 13 | 0.58 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG23 | 13 | 0.58 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG21 | 13 | 0.58 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG22 | 13 | 0.58 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG23 | 13 | 0.58 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG21 | 13 | 0.58 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG22 | 13 | 0.58 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG23 | 13 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 14 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 14 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 14 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 14 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 14 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 14 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 14 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 14 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 14 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 20 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 20 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 20 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 20 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 20 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 20 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 20 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 20 | 0.58 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 20 | 0.58 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 17 | 0.58 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 2 | 0.58 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 2 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 2 | 0.58 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 5 | 0.58 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 5 | 0.58 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 5 | 0.58 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 3 | 0.58 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 3 | 0.58 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 3 | 0.58 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 3 | 0.58 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 3 | 0.58 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 3 | 0.58 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 15 | 0.58 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 15 | 0.58 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 15 | 0.58 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 9 | 0.58 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 5 | 0.58 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 10 | 0.58 |
| (1,2315) | 1:46:A:VAL:HG21 | 1:50:A:LEU:HG | 9 | 0.58 |
| (1,2315) | 1:46:A:VAL:HG22 | 1:50:A:LEU:HG | 9 | 0.58 |
| (1,2315) | 1:46:A:VAL:HG23 | 1:50:A:LEU:HG | 9 | 0.58 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 9 | 0.58 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 1 | 0.58 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG11 | 15 | 0.58 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG12 | 15 | 0.58 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG13 | 15 | 0.58 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG21 | 15 | 0.58 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG22 | 15 | 0.58 |
| (1,2238) | 1:32:A:HIS:HB3 | 1:149:A:VAL:HG23 | 15 | 0.58 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 6 | 0.58 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 6 | 0.58 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 18 | 0.58 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 3 | 0.58 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 3 | 0.58 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 3 | 0.58 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 3 | 0.58 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 3 | 0.58 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 3 | 0.58 |
| (1,1867) | 1:37:A:GLU:HB2 | 1:38:A:GLU:HA | 5 | 0.58 |
| (1,1867) | 1:37:A:GLU:HB2 | 1:38:A:GLU:HA | 10 | 0.58 |
| (1,1759) | 1:14:A:LYS:HB2 | 1:15:A:PRO:HA | 20 | 0.58 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG2 | 5 | 0.58 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG3 | 5 | 0.58 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB2 | 17 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB3 | 17 | 0.58 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 18 | 0.58 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 18 | 0.58 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 18 | 0.58 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 1 | 0.58 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 1 | 0.58 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 1 | 0.58 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 17 | 0.58 |
| (1,1409) | 1:67:A:LEU:HB2 | 1:70:A:ASP:HB3 | 19 | 0.58 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 9 | 0.58 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 9 | 0.58 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 9 | 0.58 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 1 | 0.58 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 1 | 0.58 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 1 | 0.58 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 12 | 0.58 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 12 | 0.58 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 12 | 0.58 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 4 | 0.58 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 4 | 0.58 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 4 | 0.58 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 7 | 0.58 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 16 | 0.58 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 3 | 0.58 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 17 | 0.58 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 5 | 0.58 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 9 | 0.58 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 2 | 0.58 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 2 | 0.58 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 2 | 0.58 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 6 | 0.58 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 6 | 0.58 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 6 | 0.58 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 6 | 0.58 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 7 | 0.58 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 16 | 0.58 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 3 | 0.58 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 10 | 0.58 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 10 | 0.58 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 10 | 0.58 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 20 | 0.58 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 20 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 20 | 0.58 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 16 | 0.58 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 16 | 0.58 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 16 | 0.58 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 11 | 0.58 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 14 | 0.58 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG11 | 8 | 0.58 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG12 | 8 | 0.58 |
| (1,397) | 1:36:A:PHE:H | 1:42:A:VAL:HG13 | 8 | 0.58 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 1 | 0.58 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 1 | 0.58 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 1 | 0.58 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 2 | 0.58 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 2 | 0.58 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 2 | 0.58 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 10 | 0.58 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 10 | 0.58 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 10 | 0.58 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 17 | 0.58 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 17 | 0.58 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 17 | 0.58 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 2 | 0.58 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 2 | 0.58 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 2 | 0.58 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 9 | 0.58 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 9 | 0.58 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 9 | 0.58 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 18 | 0.58 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 18 | 0.58 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 18 | 0.58 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 7 | 0.58 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 7 | 0.58 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 19 | 0.58 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 19 | 0.58 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 19 | 0.58 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 3 | 0.57 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 3 | 0.57 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 3 | 0.57 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 3 | 0.57 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 20 | 0.57 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 20 | 0.57 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 13 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 14 | 0.57 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 18 | 0.57 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 20 | 0.57 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 9 | 0.57 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 9 | 0.57 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 8 | 0.57 |
| (1,3277) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA3 | 11 | 0.57 |
| (1,3277) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA3 | 11 | 0.57 |
| (1,3277) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA3 | 11 | 0.57 |
| (1,3269) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA2 | 12 | 0.57 |
| (1,3269) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA2 | 12 | 0.57 |
| (1,3269) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA2 | 12 | 0.57 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 7 | 0.57 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 7 | 0.57 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 7 | 0.57 |
| (1,3012) | 1:159:A:GLN:HB2 | 1:160:A:LEU:HA | 18 | 0.57 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG11 | 16 | 0.57 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG12 | 16 | 0.57 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG13 | 16 | 0.57 |
| (1,2945) | 1:23:A:LEU:HD21 | 1:58:A:LYS:HA | 15 | 0.57 |
| (1,2945) | 1:23:A:LEU:HD22 | 1:58:A:LYS:HA | 15 | 0.57 |
| (1,2945) | 1:23:A:LEU:HD23 | 1:58:A:LYS:HA | 15 | 0.57 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 11 | 0.57 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 11 | 0.57 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 11 | 0.57 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 15 | 0.57 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 15 | 0.57 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 15 | 0.57 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 15 | 0.57 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 15 | 0.57 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 15 | 0.57 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 15 | 0.57 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 15 | 0.57 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 15 | 0.57 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE1 | 2 | 0.57 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE2 | 2 | 0.57 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE1 | 2 | 0.57 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE2 | 2 | 0.57 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE1 | 2 | 0.57 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE2 | 2 | 0.57 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 2 | 0.57 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 20 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 1 | 0.57 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG11 | 8 | 0.57 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG12 | 8 | 0.57 |
| (1,2335) | 1:36:A:PHE:HA | 1:42:A:VAL:HG13 | 8 | 0.57 |
| (1,2171) | 1:86:A:LYS:H | 1:87:A:ILE:HG12 | 1 | 0.57 |
| (1,2168) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HG2 | 1 | 0.57 |
| (1,2168) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HG2 | 1 | 0.57 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 5 | 0.57 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 5 | 0.57 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 5 | 0.57 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 16 | 0.57 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 7 | 0.57 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 14 | 0.57 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 13 | 0.57 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 5 | 0.57 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 5 | 0.57 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 5 | 0.57 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 5 | 0.57 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 5 | 0.57 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 5 | 0.57 |
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 3 | 0.57 |
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 3 | 0.57 |
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 9 | 0.57 |
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 9 | 0.57 |
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 13 | 0.57 |
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 13 | 0.57 |
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 19 | 0.57 |
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 19 | 0.57 |
| (1,1778) | 1:72:A:THR:HB | 1:73:A:GLN:HB3 | 15 | 0.57 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG12 | 4 | 0.57 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG13 | 4 | 0.57 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 18 | 0.57 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 4 | 0.57 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 4 | 0.57 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 4 | 0.57 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 9 | 0.57 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 9 | 0.57 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 3 | 0.57 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 3 | 0.57 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 3 | 0.57 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 8 | 0.57 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 8 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 8 | 0.57 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 12 | 0.57 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 12 | 0.57 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 12 | 0.57 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 12 | 0.57 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 12 | 0.57 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 12 | 0.57 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 14 | 0.57 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 14 | 0.57 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 14 | 0.57 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 2 | 0.57 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 5 | 0.57 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 9 | 0.57 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 6 | 0.57 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG21 | 17 | 0.57 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG22 | 17 | 0.57 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG23 | 17 | 0.57 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 8 | 0.57 |
| (1,904) | 1:127:A:SER:H | 1:127:A:SER:HB3 | 6 | 0.57 |
| (1,839) | 1:186:A:GLU:H | 1:186:A:GLU:HB2 | 7 | 0.57 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 13 | 0.57 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 14 | 0.57 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 15 | 0.57 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 15 | 0.57 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 15 | 0.57 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 8 | 0.57 |
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 8 | 0.57 |
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 18 | 0.57 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 4 | 0.57 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 4 | 0.57 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 4 | 0.57 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 5 | 0.57 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 5 | 0.57 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 5 | 0.57 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 19 | 0.57 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 19 | 0.57 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 19 | 0.57 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 4 | 0.57 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 3 | 0.57 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 3 | 0.57 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 3 | 0.57 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 9 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 9 | 0.57 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 9 | 0.57 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 7 | 0.57 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 7 | 0.57 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 7 | 0.57 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 9 | 0.57 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 20 | 0.57 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 20 | 0.57 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 11 | 0.56 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 11 | 0.56 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 4 | 0.56 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 4 | 0.56 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 4 | 0.56 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 4 | 0.56 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 19 | 0.56 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 19 | 0.56 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 19 | 0.56 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 19 | 0.56 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 3 | 0.56 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 3 | 0.56 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 3 | 0.56 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 3 | 0.56 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 3 | 0.56 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 3 | 0.56 |
| (1,3481) | 1:29:A:TYR:HE1 | 1:67:A:LEU:HA | 10 | 0.56 |
| (1,3481) | 1:29:A:TYR:HE2 | 1:67:A:LEU:HA | 10 | 0.56 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 3 | 0.56 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 5 | 0.56 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 16 | 0.56 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 1 | 0.56 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 1 | 0.56 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 11 | 0.56 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 5 | 0.56 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 5 | 0.56 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 4 | 0.56 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 4 | 0.56 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 4 | 0.56 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 14 | 0.56 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 14 | 0.56 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 14 | 0.56 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 14 | 0.56 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 14 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 14 | 0.56 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 14 | 0.56 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 14 | 0.56 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 14 | 0.56 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 20 | 0.56 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 20 | 0.56 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 20 | 0.56 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 18 | 0.56 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 18 | 0.56 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 18 | 0.56 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 2 | 0.56 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 2 | 0.56 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 2 | 0.56 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 4 | 0.56 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 4 | 0.56 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 4 | 0.56 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 9 | 0.56 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 9 | 0.56 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 9 | 0.56 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 9 | 0.56 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 9 | 0.56 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 9 | 0.56 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 9 | 0.56 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 9 | 0.56 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 9 | 0.56 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 6 | 0.56 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 6 | 0.56 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 6 | 0.56 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 9 | 0.56 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 9 | 0.56 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 9 | 0.56 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 6 | 0.56 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 6 | 0.56 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 6 | 0.56 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 9 | 0.56 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 9 | 0.56 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 9 | 0.56 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 19 | 0.56 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 19 | 0.56 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 19 | 0.56 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 12 | 0.56 |
| (1,2334) | 1:3:A:ILE:HA | 1:8:A:GLN:HG3 | 7 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2316) | 1:117:A:LYS:H | 1:117:A:LYS:HG2 | 3 | 0.56 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 16 | 0.56 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 16 | 0.56 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 16 | 0.56 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 16 | 0.56 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 16 | 0.56 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 16 | 0.56 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 8 | 0.56 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 9 | 0.56 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 10 | 0.56 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 20 | 0.56 |
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 2 | 0.56 |
| (1,1867) | 1:37:A:GLU:HB2 | 1:38:A:GLU:HA | 6 | 0.56 |
| (1,1867) | 1:37:A:GLU:HB2 | 1:38:A:GLU:HA | 8 | 0.56 |
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 11 | 0.56 |
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 11 | 0.56 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 2 | 0.56 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 2 | 0.56 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 2 | 0.56 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 2 | 0.56 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 2 | 0.56 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 2 | 0.56 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 5 | 0.56 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 5 | 0.56 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 5 | 0.56 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 5 | 0.56 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 5 | 0.56 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 5 | 0.56 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG12 | 1 | 0.56 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG13 | 1 | 0.56 |
| (1,1697) | 1:132:A:SER:HB2 | 1:136:A:GLN:HG2 | 10 | 0.56 |
| (1,1697) | 1:132:A:SER:HB3 | 1:136:A:GLN:HG2 | 10 | 0.56 |
| (1,1697) | 1:132:A:SER:HB2 | 1:136:A:GLN:HG2 | 15 | 0.56 |
| (1,1697) | 1:132:A:SER:HB3 | 1:136:A:GLN:HG2 | 15 | 0.56 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 19 | 0.56 |
| (1,1578) | 1:118:A:GLY:H | 1:119:A:GLU:HG3 | 6 | 0.56 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 19 | 0.56 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 19 | 0.56 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 19 | 0.56 |
| (1,1547) | 1:152:A:MET:HB3 | 1:160:A:LEU:HD11 | 1 | 0.56 |
| (1,1547) | 1:152:A:MET:HB3 | 1:160:A:LEU:HD12 | 1 | 0.56 |
| (1,1547) | 1:152:A:MET:HB3 | 1:160:A:LEU:HD13 | 1 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1547) | 1:152:A:MET:HB3 | 1:160:A:LEU:HD11 | 15 | 0.56 |
| (1,1547) | 1:152:A:MET:HB3 | 1:160:A:LEU:HD12 | 15 | 0.56 |
| (1,1547) | 1:152:A:MET:HB3 | 1:160:A:LEU:HD13 | 15 | 0.56 |
| (1,1545) | 1:186:A:GLU:HG3 | 1:187:A:LYS:HD3 | 7 | 0.56 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 8 | 0.56 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 14 | 0.56 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 19 | 0.56 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 19 | 0.56 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 19 | 0.56 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG11 | 11 | 0.56 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG12 | 11 | 0.56 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG13 | 11 | 0.56 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 7 | 0.56 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 7 | 0.56 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 7 | 0.56 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 15 | 0.56 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 15 | 0.56 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 15 | 0.56 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 6 | 0.56 |
| (1,1298) | 1:141:A:ALA:HA | 1:146:A:LEU:HB2 | 13 | 0.56 |
| (1,1059) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HG3 | 7 | 0.56 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 17 | 0.56 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 18 | 0.56 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 17 | 0.56 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 7 | 0.56 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 17 | 0.56 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 9 | 0.56 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 9 | 0.56 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 9 | 0.56 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 13 | 0.56 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 13 | 0.56 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 13 | 0.56 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 18 | 0.56 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 3 | 0.56 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 3 | 0.56 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 3 | 0.56 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 11 | 0.56 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 11 | 0.56 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 11 | 0.56 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 13 | 0.56 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 13 | 0.56 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 13 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,67) | 1:26:A:PHE:H | 1:59:A:TYR:H | 20 | 0.56 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 8 | 0.55 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 8 | 0.55 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 8 | 0.55 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 8 | 0.55 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 8 | 0.55 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 8 | 0.55 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 20 | 0.55 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 20 | 0.55 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 7 | 0.55 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 7 | 0.55 |
| (1,3311) | 1:29:A:TYR:HD1 | 1:71:A:LEU:HB2 | 2 | 0.55 |
| (1,3311) | 1:29:A:TYR:HD2 | 1:71:A:LEU:HB2 | 2 | 0.55 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 6 | 0.55 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 6 | 0.55 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 6 | 0.55 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG21 | 15 | 0.55 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG22 | 15 | 0.55 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG23 | 15 | 0.55 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG21 | 15 | 0.55 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG22 | 15 | 0.55 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG23 | 15 | 0.55 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG21 | 15 | 0.55 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG22 | 15 | 0.55 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG23 | 15 | 0.55 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 13 | 0.55 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 13 | 0.55 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 13 | 0.55 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG11 | 19 | 0.55 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG12 | 19 | 0.55 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG13 | 19 | 0.55 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 3 | 0.55 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 3 | 0.55 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 3 | 0.55 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 3 | 0.55 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 3 | 0.55 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 3 | 0.55 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 3 | 0.55 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 3 | 0.55 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 3 | 0.55 |
| (1,2956) | 1:26:A:PHE:HB3 | 1:27:A:SER:HA | 13 | 0.55 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 18 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 18 | 0.55 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 18 | 0.55 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 19 | 0.55 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 19 | 0.55 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 19 | 0.55 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 5 | 0.55 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 5 | 0.55 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 5 | 0.55 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 10 | 0.55 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 10 | 0.55 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 10 | 0.55 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 2 | 0.55 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 2 | 0.55 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 2 | 0.55 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 11 | 0.55 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 11 | 0.55 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 11 | 0.55 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 13 | 0.55 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 13 | 0.55 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 13 | 0.55 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 14 | 0.55 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 14 | 0.55 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 14 | 0.55 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 16 | 0.55 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 16 | 0.55 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 16 | 0.55 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 4 | 0.55 |
| (1,2357) | 1:184:A:LEU:HA | 1:187:A:LYS:HG2 | 7 | 0.55 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 8 | 0.55 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 8 | 0.55 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 8 | 0.55 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 11 | 0.55 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 10 | 0.55 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 10 | 0.55 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 6 | 0.55 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 6 | 0.55 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 6 | 0.55 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 6 | 0.55 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 6 | 0.55 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 6 | 0.55 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 9 | 0.55 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 9 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 9 | 0.55 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 15 | 0.55 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 11 | 0.55 |
| (1,2016) | 1:117:A:LYS:HD3 | 1:119:A:GLU:H | 12 | 0.55 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 1 | 0.55 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 1 | 0.55 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 1 | 0.55 |
| (1,1931) | 1:62:A:GLU:HB2 | 1:63:A:PHE:HB3 | 4 | 0.55 |
| (1,1931) | 1:62:A:GLU:HB3 | 1:63:A:PHE:HB3 | 4 | 0.55 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 3 | 0.55 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 5 | 0.55 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 15 | 0.55 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 19 | 0.55 |
| (1,1867) | 1:37:A:GLU:HB2 | 1:38:A:GLU:HA | 12 | 0.55 |
| (1,1867) | 1:37:A:GLU:HB2 | 1:38:A:GLU:HA | 16 | 0.55 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 19 | 0.55 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 19 | 0.55 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 19 | 0.55 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 19 | 0.55 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 19 | 0.55 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 19 | 0.55 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 12 | 0.55 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 12 | 0.55 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 12 | 0.55 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 9 | 0.55 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 10 | 0.55 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 4 | 0.55 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 19 | 0.55 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 14 | 0.55 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 14 | 0.55 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 14 | 0.55 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 14 | 0.55 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 14 | 0.55 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 14 | 0.55 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 18 | 0.55 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 18 | 0.55 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 18 | 0.55 |
| (1,1363) | 1:97:A:LYS:HE2 | 1:98:A:THR:H | 10 | 0.55 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE2 | 7 | 0.55 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE3 | 7 | 0.55 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE2 | 7 | 0.55 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE3 | 7 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE2 | 7 | 0.55 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE3 | 7 | 0.55 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 20 | 0.55 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 5 | 0.55 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 5 | 0.55 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 5 | 0.55 |
| (1,1331) | 1:70:A:ASP:HB3 | 1:72:A:THR:H | 2 | 0.55 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB2 | 18 | 0.55 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB3 | 18 | 0.55 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB2 | 19 | 0.55 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB3 | 19 | 0.55 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 8 | 0.55 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 13 | 0.55 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 19 | 0.55 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 18 | 0.55 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 1 | 0.55 |
| (1,991) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HD22 | 16 | 0.55 |
| (1,883) | 1:49:A:LYS:H | 1:49:A:LYS:HD3 | 11 | 0.55 |
| (1,765) | 1:106:A:ASP:H | 1:106:A:ASP:HB3 | 7 | 0.55 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 1 | 0.55 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG11 | 2 | 0.55 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG12 | 2 | 0.55 |
| (1,740) | 1:35:A:GLN:H | 1:39:A:VAL:HG13 | 2 | 0.55 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 4 | 0.55 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 15 | 0.55 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 15 | 0.55 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 15 | 0.55 |
| (1,530) | 1:128:A:PHE:HB3 | 1:129:A:VAL:H | 9 | 0.55 |
| (1,530) | 1:128:A:PHE:HB3 | 1:129:A:VAL:H | 11 | 0.55 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 8 | 0.55 |
| (1,438) | 1:60:A:HIS:HB2 | 1:75:A:TRP:H | 19 | 0.55 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 7 | 0.55 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 7 | 0.55 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 7 | 0.55 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 17 | 0.55 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 17 | 0.55 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 17 | 0.55 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 18 | 0.55 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 18 | 0.55 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 18 | 0.55 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 13 | 0.55 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 13 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 10 | 0.55 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 10 | 0.55 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 10 | 0.55 |
| (1,83) | 1:6:A:GLY:H | 1:11:A:THR:H | 12 | 0.55 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE1 | 4 | 0.54 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE2 | 4 | 0.54 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE1 | 4 | 0.54 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE2 | 4 | 0.54 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE1 | 4 | 0.54 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE2 | 4 | 0.54 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 8 | 0.54 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 8 | 0.54 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 2 | 0.54 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 2 | 0.54 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 2 | 0.54 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 2 | 0.54 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 20 | 0.54 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 20 | 0.54 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 3 | 0.54 |
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 8 | 0.54 |
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 8 | 0.54 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 16 | 0.54 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 16 | 0.54 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 4 | 0.54 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 4 | 0.54 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 8 | 0.54 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 8 | 0.54 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 20 | 0.54 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 20 | 0.54 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 20 | 0.54 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 20 | 0.54 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 20 | 0.54 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 20 | 0.54 |
| (1,3277) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA3 | 12 | 0.54 |
| (1,3277) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA3 | 12 | 0.54 |
| (1,3277) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA3 | 12 | 0.54 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 12 | 0.54 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 12 | 0.54 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 12 | 0.54 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 14 | 0.54 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 14 | 0.54 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 14 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3112) | 1:67:A:LEU:HA | 1:70:A:ASP:HB3 | 14 | 0.54 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 17 | 0.54 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 17 | 0.54 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 17 | 0.54 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 17 | 0.54 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 17 | 0.54 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 17 | 0.54 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 17 | 0.54 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 17 | 0.54 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 17 | 0.54 |
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 6 | 0.54 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 6 | 0.54 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 6 | 0.54 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 13 | 0.54 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 13 | 0.54 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 13 | 0.54 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 17 | 0.54 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 17 | 0.54 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 17 | 0.54 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 9 | 0.54 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 9 | 0.54 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 9 | 0.54 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 8 | 0.54 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 14 | 0.54 |
| (1,2771) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HG | 17 | 0.54 |
| (1,2771) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HG | 17 | 0.54 |
| (1,2771) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HG | 17 | 0.54 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 7 | 0.54 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 7 | 0.54 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 7 | 0.54 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 7 | 0.54 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 7 | 0.54 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 7 | 0.54 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 20 | 0.54 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 20 | 0.54 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 20 | 0.54 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 20 | 0.54 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 20 | 0.54 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 20 | 0.54 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 8 | 0.54 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 8 | 0.54 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 8 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 9 | 0.54 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 9 | 0.54 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 9 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG21 | 2 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG22 | 2 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG23 | 2 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG21 | 2 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG22 | 2 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG23 | 2 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG21 | 9 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG22 | 9 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG23 | 9 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG21 | 9 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG22 | 9 | 0.54 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG23 | 9 | 0.54 |
| (1,2631) | 1:101:A:VAL:HG21 | 1:103:A:SER:H | 17 | 0.54 |
| (1,2631) | 1:101:A:VAL:HG22 | 1:103:A:SER:H | 17 | 0.54 |
| (1,2631) | 1:101:A:VAL:HG23 | 1:103:A:SER:H | 17 | 0.54 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 10 | 0.54 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 10 | 0.54 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 10 | 0.54 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 10 | 0.54 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 10 | 0.54 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 10 | 0.54 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 10 | 0.54 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 10 | 0.54 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 10 | 0.54 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 12 | 0.54 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 12 | 0.54 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 12 | 0.54 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 2 | 0.54 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 9 | 0.54 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 14 | 0.54 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 14 | 0.54 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 14 | 0.54 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 15 | 0.54 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 10 | 0.54 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 10 | 0.54 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 10 | 0.54 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 14 | 0.54 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 14 | 0.54 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 14 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 14 | 0.54 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 14 | 0.54 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 14 | 0.54 |
| (1,2171) | 1:86:A:LYS:H | 1:87:A:ILE:HG12 | 2 | 0.54 |
| (1,2168) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HG2 | 15 | 0.54 |
| (1,2168) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HG2 | 15 | 0.54 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 18 | 0.54 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 18 | 0.54 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 18 | 0.54 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 1 | 0.54 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 4 | 0.54 |
| (1,2055) | 1:118:A:GLY:H | 1:119:A:GLU:HB2 | 16 | 0.54 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 12 | 0.54 |
| (1,1825) | 1:117:A:LYS:HB3 | 1:120:A:ASP:H | 7 | 0.54 |
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 5 | 0.54 |
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 5 | 0.54 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 8 | 0.54 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 19 | 0.54 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 19 | 0.54 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 19 | 0.54 |
| (1,1588) | 1:62:A:GLU:HA | 1:62:A:GLU:HG3 | 14 | 0.54 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 13 | 0.54 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 13 | 0.54 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 13 | 0.54 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 9 | 0.54 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 9 | 0.54 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 9 | 0.54 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 19 | 0.54 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 19 | 0.54 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 19 | 0.54 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 4 | 0.54 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 4 | 0.54 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 4 | 0.54 |
| (1,1409) | 1:67:A:LEU:HB2 | 1:70:A:ASP:HB3 | 20 | 0.54 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 7 | 0.54 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 7 | 0.54 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 7 | 0.54 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 15 | 0.54 |
| (1,1134) | 1:73:A:GLN:HE21 | 1:126:A:ASN:H | 13 | 0.54 |
| (1,1080) | 1:34:A:TYR:HD2 | 1:38:A:GLU:H | 10 | 0.54 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 3 | 0.54 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 4 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 15 | 0.54 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 9 | 0.54 |
| (1,894) | 1:103:A:SER:H | 1:106:A:ASP:HB3 | 7 | 0.54 |
| (1,894) | 1:103:A:SER:H | 1:106:A:ASP:HB3 | 11 | 0.54 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 1 | 0.54 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 1 | 0.54 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 1 | 0.54 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 17 | 0.54 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 17 | 0.54 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 17 | 0.54 |
| (1,530) | 1:128:A:PHE:HB3 | 1:129:A:VAL:H | 3 | 0.54 |
| (1,530) | 1:128:A:PHE:HB3 | 1:129:A:VAL:H | 5 | 0.54 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 20 | 0.54 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 5 | 0.54 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 5 | 0.54 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 5 | 0.54 |
| (1,441) | 1:34:A:TYR:HE2 | 1:92:A:PHE:H | 7 | 0.54 |
| (1,416) | 1:122:A:ASP:HB3 | 1:123:A:ALA:H | 2 | 0.54 |
| (1,259) | 1:69:A:LYS:HD2 | 1:70:A:ASP:H | 11 | 0.54 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 7 | 0.54 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 7 | 0.54 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 7 | 0.54 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 9 | 0.54 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 9 | 0.54 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 9 | 0.54 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 12 | 0.54 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 12 | 0.54 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 12 | 0.54 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 13 | 0.54 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 13 | 0.54 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 13 | 0.54 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 20 | 0.54 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 20 | 0.54 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 20 | 0.54 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 11 | 0.54 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 11 | 0.54 |
| (1,128) | 1:12:A:LEU:HD11 | 1:159:A:GLN:H | 1 | 0.54 |
| (1,128) | 1:12:A:LEU:HD12 | 1:159:A:GLN:H | 1 | 0.54 |
| (1,128) | 1:12:A:LEU:HD13 | 1:159:A:GLN:H | 1 | 0.54 |
| (1,127) | 1:105:A:ALA:H | 1:107:A:ILE:HB | 11 | 0.54 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 3 | 0.54 |
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 8 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 4 | 0.53 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 4 | 0.53 |
| (1,3480) | 1:32:A:HIS:HD2 | 1:150:A:PRO:HG3 | 5 | 0.53 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 2 | 0.53 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 10 | 0.53 |
| (1,3338) | 1:38:A:GLU:HG3 | 1:92:A:PHE:HD1 | 14 | 0.53 |
| (1,3338) | 1:38:A:GLU:HG3 | 1:92:A:PHE:HD2 | 14 | 0.53 |
| (1,3311) | 1:29:A:TYR:HD1 | 1:71:A:LEU:HB2 | 11 | 0.53 |
| (1,3311) | 1:29:A:TYR:HD2 | 1:71:A:LEU:HB2 | 11 | 0.53 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 2 | 0.53 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 2 | 0.53 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 2 | 0.53 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 2 | 0.53 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 2 | 0.53 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 2 | 0.53 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB2 | 13 | 0.53 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB3 | 13 | 0.53 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 17 | 0.53 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 17 | 0.53 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 17 | 0.53 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE1 | 13 | 0.53 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE2 | 13 | 0.53 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE3 | 13 | 0.53 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE1 | 15 | 0.53 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE2 | 15 | 0.53 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE3 | 15 | 0.53 |
| (1,2935) | 1:75:A:TRP:HA | 1:78:A:ALA:HA | 13 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 4 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 4 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 4 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 5 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 5 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 5 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 6 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 6 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 6 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 15 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 15 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 15 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 18 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 18 | 0.53 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 18 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 5 | 0.53 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 2 | 0.53 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 2 | 0.53 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 2 | 0.53 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 17 | 0.53 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 17 | 0.53 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 17 | 0.53 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 19 | 0.53 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 19 | 0.53 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 19 | 0.53 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 3 | 0.53 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 3 | 0.53 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 3 | 0.53 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 18 | 0.53 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 18 | 0.53 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 18 | 0.53 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 18 | 0.53 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 18 | 0.53 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 18 | 0.53 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 18 | 0.53 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 18 | 0.53 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 18 | 0.53 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 2 | 0.53 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 2 | 0.53 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 2 | 0.53 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 20 | 0.53 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 20 | 0.53 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 20 | 0.53 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 20 | 0.53 |
| (1,2464) | 1:108:A:ARG:HG3 | 1:109:A:LYS:HA | 9 | 0.53 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 4 | 0.53 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 4 | 0.53 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 4 | 0.53 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 4 | 0.53 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 4 | 0.53 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 4 | 0.53 |
| (1,2452) | 1:149:A:VAL:HG11 | 1:150:A:PRO:HG3 | 5 | 0.53 |
| (1,2452) | 1:149:A:VAL:HG12 | 1:150:A:PRO:HG3 | 5 | 0.53 |
| (1,2452) | 1:149:A:VAL:HG13 | 1:150:A:PRO:HG3 | 5 | 0.53 |
| (1,2452) | 1:149:A:VAL:HG21 | 1:150:A:PRO:HG3 | 5 | 0.53 |
| (1,2452) | 1:149:A:VAL:HG22 | 1:150:A:PRO:HG3 | 5 | 0.53 |
| (1,2452) | 1:149:A:VAL:HG23 | 1:150:A:PRO:HG3 | 5 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 10 | 0.53 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 3 | 0.53 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 3 | 0.53 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 3 | 0.53 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 14 | 0.53 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 14 | 0.53 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 14 | 0.53 |
| (1,2291) | 1:117:A:LYS:HG3 | 1:120:A:ASP:H | 4 | 0.53 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 13 | 0.53 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 13 | 0.53 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 13 | 0.53 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 18 | 0.53 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 18 | 0.53 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 18 | 0.53 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 2 | 0.53 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 2 | 0.53 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 2 | 0.53 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 2 | 0.53 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 2 | 0.53 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 2 | 0.53 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 13 | 0.53 |
| (1,1965) | 1:34:A:TYR:HA | 1:38:A:GLU:HB3 | 15 | 0.53 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 7 | 0.53 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 14 | 0.53 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 12 | 0.53 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 12 | 0.53 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 12 | 0.53 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 12 | 0.53 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 12 | 0.53 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 12 | 0.53 |
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 20 | 0.53 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD1 | 6 | 0.53 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD2 | 6 | 0.53 |
| (1,1686) | 1:99:A:GLN:HG3 | 1:100:A:THR:H | 1 | 0.53 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 6 | 0.53 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 8 | 0.53 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 8 | 0.53 |
| (1,1606) | 1:52:A:GLU:HG2 | 1:53:A:GLY:HA3 | 13 | 0.53 |
| (1,1606) | 1:52:A:GLU:HG3 | 1:53:A:GLY:HA3 | 13 | 0.53 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 11 | 0.53 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 2 | 0.53 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 2 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 2 | 0.53 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 6 | 0.53 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 6 | 0.53 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 6 | 0.53 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 11 | 0.53 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 5 | 0.53 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 5 | 0.53 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 5 | 0.53 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 14 | 0.53 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 14 | 0.53 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 14 | 0.53 |
| (1,1432) | 1:85:A:ASP:HB3 | 1:86:A:LYS:HG2 | 9 | 0.53 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 3 | 0.53 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 1 | 0.53 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 11 | 0.53 |
| (1,1191) | 1:64:A:LEU:HD11 | 1:65:A:GLY:H | 2 | 0.53 |
| (1,1191) | 1:64:A:LEU:HD12 | 1:65:A:GLY:H | 2 | 0.53 |
| (1,1191) | 1:64:A:LEU:HD13 | 1:65:A:GLY:H | 2 | 0.53 |
| (1,1134) | 1:73:A:GLN:HE21 | 1:126:A:ASN:H | 16 | 0.53 |
| (1,991) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HD22 | 5 | 0.53 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 11 | 0.53 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 11 | 0.53 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 11 | 0.53 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 12 | 0.53 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 12 | 0.53 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 12 | 0.53 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 13 | 0.53 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 14 | 0.53 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 14 | 0.53 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 14 | 0.53 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG21 | 11 | 0.53 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG22 | 11 | 0.53 |
| (1,631) | 1:91:A:MET:H | 1:110:A:VAL:HG23 | 11 | 0.53 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 8 | 0.53 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 8 | 0.53 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 8 | 0.53 |
| (1,438) | 1:60:A:HIS:HB2 | 1:75:A:TRP:H | 5 | 0.53 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 6 | 0.53 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 6 | 0.53 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 6 | 0.53 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG11 | 19 | 0.53 |
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG12 | 19 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,352) | 1:112:A:VAL:H | 1:112:A:VAL:HG13 | 19 | 0.53 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 18 | 0.53 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 18 | 0.53 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 18 | 0.53 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 3 | 0.53 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 3 | 0.53 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 3 | 0.53 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 8 | 0.53 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 8 | 0.53 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 8 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 1 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 1 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 1 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 2 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 2 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 2 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 4 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 4 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 4 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 6 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 6 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 6 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 11 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 11 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 11 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 15 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 15 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 15 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 16 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 16 | 0.53 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 16 | 0.53 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 1 | 0.53 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 1 | 0.53 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 5 | 0.53 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 5 | 0.53 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 20 | 0.53 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 20 | 0.53 |
| (1,102) | 1:50:A:LEU:HD21 | 1:56:A:MET:H | 20 | 0.53 |
| (1,102) | 1:50:A:LEU:HD22 | 1:56:A:MET:H | 20 | 0.53 |
| (1,102) | 1:50:A:LEU:HD23 | 1:56:A:MET:H | 20 | 0.53 |
| (1,90) | 1:185:A:VAL:HA | 1:188:A:LYS:H | 2 | 0.53 |
| (1,83) | 1:6:A:GLY:H | 1:11:A:THR:H | 16 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 12 | 0.52 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 7 | 0.52 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 3 | 0.52 |
| (1,3415) | 1:59:A:TYR:HD1 | 1:137:A:GLN:HG3 | 5 | 0.52 |
| (1,3415) | 1:59:A:TYR:HD2 | 1:137:A:GLN:HG3 | 5 | 0.52 |
| (1,3277) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA3 | 15 | 0.52 |
| (1,3277) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA3 | 15 | 0.52 |
| (1,3277) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA3 | 15 | 0.52 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 3 | 0.52 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 3 | 0.52 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 3 | 0.52 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 16 | 0.52 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 16 | 0.52 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 16 | 0.52 |
| (1,3112) | 1:67:A:LEU:HA | 1:70:A:ASP:HB3 | 13 | 0.52 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 5 | 0.52 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 5 | 0.52 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 5 | 0.52 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD21 | 5 | 0.52 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD22 | 5 | 0.52 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD23 | 5 | 0.52 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 4 | 0.52 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 4 | 0.52 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 4 | 0.52 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 3 | 0.52 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 3 | 0.52 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 3 | 0.52 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 9 | 0.52 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 9 | 0.52 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 9 | 0.52 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 5 | 0.52 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 5 | 0.52 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 5 | 0.52 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 12 | 0.52 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 12 | 0.52 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 12 | 0.52 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 15 | 0.52 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 15 | 0.52 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 15 | 0.52 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 18 | 0.52 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 18 | 0.52 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 18 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 11 | 0.52 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 12 | 0.52 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE1 | 12 | 0.52 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE2 | 12 | 0.52 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE1 | 12 | 0.52 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE2 | 12 | 0.52 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE1 | 12 | 0.52 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE2 | 12 | 0.52 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 7 | 0.52 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 9 | 0.52 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 9 | 0.52 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 9 | 0.52 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 12 | 0.52 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 12 | 0.52 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 12 | 0.52 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 19 | 0.52 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 19 | 0.52 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 19 | 0.52 |
| (1,2171) | 1:86:A:LYS:H | 1:87:A:ILE:HG12 | 3 | 0.52 |
| (1,2168) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HG2 | 6 | 0.52 |
| (1,2168) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HG2 | 6 | 0.52 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 3 | 0.52 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 8 | 0.52 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 11 | 0.52 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 16 | 0.52 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 17 | 0.52 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 20 | 0.52 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 7 | 0.52 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 9 | 0.52 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 11 | 0.52 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 14 | 0.52 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 14 | 0.52 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 14 | 0.52 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 14 | 0.52 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 14 | 0.52 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 14 | 0.52 |
| (1,1867) | 1:37:A:GLU:HB2 | 1:38:A:GLU:HA | 1 | 0.52 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 13 | 0.52 |
| (1,1813) | 1:160:A:LEU:HD21 | 1:180:A:THR:HB | 16 | 0.52 |
| (1,1813) | 1:160:A:LEU:HD22 | 1:180:A:THR:HB | 16 | 0.52 |
| (1,1813) | 1:160:A:LEU:HD23 | 1:180:A:THR:HB | 16 | 0.52 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 1 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 1 | 0.52 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 1 | 0.52 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 1 | 0.52 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 1 | 0.52 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 1 | 0.52 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 13 | 0.52 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 13 | 0.52 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 13 | 0.52 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 13 | 0.52 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 13 | 0.52 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 13 | 0.52 |
| (1,1697) | 1:132:A:SER:HB2 | 1:136:A:GLN:HG2 | 5 | 0.52 |
| (1,1697) | 1:132:A:SER:HB3 | 1:136:A:GLN:HG2 | 5 | 0.52 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 10 | 0.52 |
| (1,1606) | 1:52:A:GLU:HG2 | 1:53:A:GLY:HA3 | 10 | 0.52 |
| (1,1606) | 1:52:A:GLU:HG3 | 1:53:A:GLY:HA3 | 10 | 0.52 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 5 | 0.52 |
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 19 | 0.52 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 19 | 0.52 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 19 | 0.52 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 1 | 0.52 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 5 | 0.52 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 16 | 0.52 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 15 | 0.52 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 15 | 0.52 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 15 | 0.52 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 7 | 0.52 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 7 | 0.52 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 7 | 0.52 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 15 | 0.52 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 15 | 0.52 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 15 | 0.52 |
| (1,1409) | 1:67:A:LEU:HB2 | 1:70:A:ASP:HB3 | 9 | 0.52 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 3 | 0.52 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 3 | 0.52 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 3 | 0.52 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 7 | 0.52 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 7 | 0.52 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 7 | 0.52 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG11 | 8 | 0.52 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG12 | 8 | 0.52 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG13 | 8 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 1 | 0.52 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 5 | 0.52 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 11 | 0.52 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 13 | 0.52 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 3 | 0.52 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 19 | 0.52 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 17 | 0.52 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 17 | 0.52 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 17 | 0.52 |
| (1,765) | 1:106:A:ASP:H | 1:106:A:ASP:HB3 | 9 | 0.52 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 6 | 0.52 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 14 | 0.52 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 14 | 0.52 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 14 | 0.52 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 18 | 0.52 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 18 | 0.52 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 18 | 0.52 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 12 | 0.52 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 1 | 0.52 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 1 | 0.52 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 1 | 0.52 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 3 | 0.52 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 3 | 0.52 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 3 | 0.52 |
| (1,441) | 1:34:A:TYR:HE1 | 1:92:A:PHE:H | 13 | 0.52 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 6 | 0.52 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 17 | 0.52 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 17 | 0.52 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 17 | 0.52 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 17 | 0.52 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 19 | 0.52 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 19 | 0.52 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 19 | 0.52 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 3 | 0.52 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 3 | 0.52 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 9 | 0.52 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 9 | 0.52 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 12 | 0.52 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 12 | 0.52 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 16 | 0.52 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 16 | 0.52 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 8 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 8 | 0.52 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 8 | 0.52 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 7 | 0.52 |
| (1,90) | 1:185:A:VAL:HA | 1:188:A:LYS:H | 17 | 0.52 |
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 1 | 0.52 |
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 20 | 0.52 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE1 | 17 | 0.51 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE2 | 17 | 0.51 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE1 | 17 | 0.51 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE2 | 17 | 0.51 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE1 | 17 | 0.51 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE2 | 17 | 0.51 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB2 | 11 | 0.51 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB3 | 11 | 0.51 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB2 | 11 | 0.51 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB3 | 11 | 0.51 |
| (1,3481) | 1:29:A:TYR:HE1 | 1:67:A:LEU:HA | 8 | 0.51 |
| (1,3481) | 1:29:A:TYR:HE2 | 1:67:A:LEU:HA | 8 | 0.51 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 8 | 0.51 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 18 | 0.51 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 15 | 0.51 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 18 | 0.51 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 18 | 0.51 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 10 | 0.51 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 10 | 0.51 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 10 | 0.51 |
| (1,3112) | 1:67:A:LEU:HA | 1:70:A:ASP:HB3 | 15 | 0.51 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG11 | 16 | 0.51 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG12 | 16 | 0.51 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG13 | 16 | 0.51 |
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 10 | 0.51 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 10 | 0.51 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 10 | 0.51 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 18 | 0.51 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 16 | 0.51 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 16 | 0.51 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 16 | 0.51 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 12 | 0.51 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 12 | 0.51 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 12 | 0.51 |
| (1,2838) | 1:34:A:TYR:HE1 | 1:38:A:GLU:HA | 8 | 0.51 |
| (1,2838) | 1:34:A:TYR:HE2 | 1:38:A:GLU:HA | 8 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 7 | 0.51 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 7 | 0.51 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 7 | 0.51 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 4 | 0.51 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 4 | 0.51 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 4 | 0.51 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 4 | 0.51 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 4 | 0.51 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 4 | 0.51 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 5 | 0.51 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 5 | 0.51 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 5 | 0.51 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 6 | 0.51 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 6 | 0.51 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 6 | 0.51 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 10 | 0.51 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 10 | 0.51 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 10 | 0.51 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 20 | 0.51 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 20 | 0.51 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 20 | 0.51 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG21 | 4 | 0.51 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG22 | 4 | 0.51 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG23 | 4 | 0.51 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG21 | 4 | 0.51 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG22 | 4 | 0.51 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG23 | 4 | 0.51 |
| (1,2512) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HB2 | 16 | 0.51 |
| (1,2512) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HB2 | 16 | 0.51 |
| (1,2512) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HB2 | 16 | 0.51 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 5 | 0.51 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 5 | 0.51 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 5 | 0.51 |
| (1,2456) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HA | 10 | 0.51 |
| (1,2456) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HA | 10 | 0.51 |
| (1,2456) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HA | 10 | 0.51 |
| (1,2452) | 1:149:A:VAL:HG11 | 1:150:A:PRO:HG3 | 6 | 0.51 |
| (1,2452) | 1:149:A:VAL:HG12 | 1:150:A:PRO:HG3 | 6 | 0.51 |
| (1,2452) | 1:149:A:VAL:HG13 | 1:150:A:PRO:HG3 | 6 | 0.51 |
| (1,2452) | 1:149:A:VAL:HG21 | 1:150:A:PRO:HG3 | 6 | 0.51 |
| (1,2452) | 1:149:A:VAL:HG22 | 1:150:A:PRO:HG3 | 6 | 0.51 |
| (1,2452) | 1:149:A:VAL:HG23 | 1:150:A:PRO:HG3 | 6 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 8 | 0.51 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 13 | 0.51 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 13 | 0.51 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 13 | 0.51 |
| (1,2291) | 1:117:A:LYS:HG3 | 1:120:A:ASP:H | 3 | 0.51 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 17 | 0.51 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 17 | 0.51 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 17 | 0.51 |
| (1,2283) | 1:128:A:PHE:HA | 1:131:A:LYS:HD3 | 5 | 0.51 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 18 | 0.51 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 8 | 0.51 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 8 | 0.51 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 8 | 0.51 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 8 | 0.51 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 8 | 0.51 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 8 | 0.51 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 15 | 0.51 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 15 | 0.51 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 15 | 0.51 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 15 | 0.51 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 15 | 0.51 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 15 | 0.51 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG11 | 15 | 0.51 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG12 | 15 | 0.51 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG13 | 15 | 0.51 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 1 | 0.51 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 5 | 0.51 |
| (1,1931) | 1:62:A:GLU:HB2 | 1:63:A:PHE:HB3 | 9 | 0.51 |
| (1,1931) | 1:62:A:GLU:HB3 | 1:63:A:PHE:HB3 | 9 | 0.51 |
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 12 | 0.51 |
| (1,1867) | 1:37:A:GLU:HB2 | 1:38:A:GLU:HA | 11 | 0.51 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 6 | 0.51 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 4 | 0.51 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 4 | 0.51 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 4 | 0.51 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 4 | 0.51 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 4 | 0.51 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 4 | 0.51 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 17 | 0.51 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 17 | 0.51 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 17 | 0.51 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 17 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 17 | 0.51 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 17 | 0.51 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 6 | 0.51 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 6 | 0.51 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 6 | 0.51 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 13 | 0.51 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 13 | 0.51 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 13 | 0.51 |
| (1,1581) | 1:62:A:GLU:HA | 1:62:A:GLU:HG2 | 1 | 0.51 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 12 | 0.51 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 12 | 0.51 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 12 | 0.51 |
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 8 | 0.51 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 8 | 0.51 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 8 | 0.51 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 6 | 0.51 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 3 | 0.51 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 3 | 0.51 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 3 | 0.51 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB2 | 12 | 0.51 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB3 | 12 | 0.51 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB2 | 13 | 0.51 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB3 | 13 | 0.51 |
| (1,1191) | 1:64:A:LEU:HD11 | 1:65:A:GLY:H | 5 | 0.51 |
| (1,1191) | 1:64:A:LEU:HD12 | 1:65:A:GLY:H | 5 | 0.51 |
| (1,1191) | 1:64:A:LEU:HD13 | 1:65:A:GLY:H | 5 | 0.51 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG11 | 4 | 0.51 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG12 | 4 | 0.51 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG13 | 4 | 0.51 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 19 | 0.51 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 19 | 0.51 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 19 | 0.51 |
| (1,1080) | 1:34:A:TYR:HD2 | 1:38:A:GLU:H | 13 | 0.51 |
| (1,991) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HD22 | 18 | 0.51 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 7 | 0.51 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 10 | 0.51 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 11 | 0.51 |
| (1,883) | 1:49:A:LYS:H | 1:49:A:LYS:HD3 | 5 | 0.51 |
| (1,883) | 1:49:A:LYS:H | 1:49:A:LYS:HD3 | 16 | 0.51 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 15 | 0.51 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 19 | 0.51 |
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 1 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 3 | 0.51 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 3 | 0.51 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 3 | 0.51 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 15 | 0.51 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 15 | 0.51 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 15 | 0.51 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 18 | 0.51 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 18 | 0.51 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 18 | 0.51 |
| (1,449) | 1:171:A:ASP:H | 1:172:A:VAL:HA | 2 | 0.51 |
| (1,438) | 1:60:A:HIS:HB2 | 1:75:A:TRP:H | 18 | 0.51 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 15 | 0.51 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 15 | 0.51 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 15 | 0.51 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 7 | 0.51 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 7 | 0.51 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 7 | 0.51 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 10 | 0.51 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 10 | 0.51 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 10 | 0.51 |
| (1,209) | 1:149:A:VAL:HG21 | 1:151:A:ALA:H | 8 | 0.51 |
| (1,209) | 1:149:A:VAL:HG22 | 1:151:A:ALA:H | 8 | 0.51 |
| (1,209) | 1:149:A:VAL:HG23 | 1:151:A:ALA:H | 8 | 0.51 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 6 | 0.51 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 18 | 0.51 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 18 | 0.51 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 18 | 0.51 |
| (1,128) | 1:12:A:LEU:HD11 | 1:159:A:GLN:H | 2 | 0.51 |
| (1,128) | 1:12:A:LEU:HD12 | 1:159:A:GLN:H | 2 | 0.51 |
| (1,128) | 1:12:A:LEU:HD13 | 1:159:A:GLN:H | 2 | 0.51 |
| (1,127) | 1:105:A:ALA:H | 1:107:A:ILE:HB | 18 | 0.51 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 8 | 0.51 |
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 11 | 0.51 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE1 | 13 | 0.5 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE2 | 13 | 0.5 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE1 | 13 | 0.5 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE2 | 13 | 0.5 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE1 | 13 | 0.5 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE2 | 13 | 0.5 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB2 | 12 | 0.5 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB3 | 12 | 0.5 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB2 | 12 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB3 | 12 | 0.5 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 2 | 0.5 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 2 | 0.5 |
| (1,3311) | 1:29:A:TYR:HD1 | 1:71:A:LEU:HB2 | 6 | 0.5 |
| (1,3311) | 1:29:A:TYR:HD2 | 1:71:A:LEU:HB2 | 6 | 0.5 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 19 | 0.5 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 19 | 0.5 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 19 | 0.5 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 19 | 0.5 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 19 | 0.5 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 19 | 0.5 |
| (1,3252) | 1:29:A:TYR:HD1 | 1:68:A:GLY:HA3 | 4 | 0.5 |
| (1,3252) | 1:29:A:TYR:HD2 | 1:68:A:GLY:HA3 | 4 | 0.5 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD21 | 14 | 0.5 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD22 | 14 | 0.5 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD23 | 14 | 0.5 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD21 | 15 | 0.5 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD22 | 15 | 0.5 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD23 | 15 | 0.5 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 13 | 0.5 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 13 | 0.5 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 13 | 0.5 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 17 | 0.5 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 17 | 0.5 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 17 | 0.5 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 1 | 0.5 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 1 | 0.5 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 1 | 0.5 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 19 | 0.5 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 19 | 0.5 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 19 | 0.5 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 20 | 0.5 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 20 | 0.5 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 20 | 0.5 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 11 | 0.5 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 11 | 0.5 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 11 | 0.5 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 12 | 0.5 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 12 | 0.5 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 12 | 0.5 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG21 | 11 | 0.5 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG22 | 11 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG23 | 11 | 0.5 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG21 | 11 | 0.5 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG22 | 11 | 0.5 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG23 | 11 | 0.5 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG21 | 18 | 0.5 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG22 | 18 | 0.5 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG23 | 18 | 0.5 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG21 | 18 | 0.5 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG22 | 18 | 0.5 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG23 | 18 | 0.5 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 13 | 0.5 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 13 | 0.5 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 13 | 0.5 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 13 | 0.5 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 13 | 0.5 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 13 | 0.5 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 13 | 0.5 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 13 | 0.5 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 13 | 0.5 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 3 | 0.5 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 3 | 0.5 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 3 | 0.5 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 6 | 0.5 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 7 | 0.5 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 10 | 0.5 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 10 | 0.5 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 10 | 0.5 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 10 | 0.5 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 13 | 0.5 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 13 | 0.5 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 13 | 0.5 |
| (1,2452) | 1:149:A:VAL:HG11 | 1:150:A:PRO:HG3 | 4 | 0.5 |
| (1,2452) | 1:149:A:VAL:HG12 | 1:150:A:PRO:HG3 | 4 | 0.5 |
| (1,2452) | 1:149:A:VAL:HG13 | 1:150:A:PRO:HG3 | 4 | 0.5 |
| (1,2452) | 1:149:A:VAL:HG21 | 1:150:A:PRO:HG3 | 4 | 0.5 |
| (1,2452) | 1:149:A:VAL:HG22 | 1:150:A:PRO:HG3 | 4 | 0.5 |
| (1,2452) | 1:149:A:VAL:HG23 | 1:150:A:PRO:HG3 | 4 | 0.5 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 3 | 0.5 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 19 | 0.5 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 3 | 0.5 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 1 | 0.5 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 1 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 1 | 0.5 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 1 | 0.5 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 1 | 0.5 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 1 | 0.5 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 16 | 0.5 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 16 | 0.5 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 16 | 0.5 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 2 | 0.5 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 13 | 0.5 |
| (1,1931) | 1:62:A:GLU:HB2 | 1:63:A:PHE:HB3 | 2 | 0.5 |
| (1,1931) | 1:62:A:GLU:HB3 | 1:63:A:PHE:HB3 | 2 | 0.5 |
| (1,1931) | 1:62:A:GLU:HB2 | 1:63:A:PHE:HB3 | 5 | 0.5 |
| (1,1931) | 1:62:A:GLU:HB3 | 1:63:A:PHE:HB3 | 5 | 0.5 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 20 | 0.5 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 20 | 0.5 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 20 | 0.5 |
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 12 | 0.5 |
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 12 | 0.5 |
| (1,1778) | 1:72:A:THR:HB | 1:73:A:GLN:HB3 | 3 | 0.5 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 3 | 0.5 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 3 | 0.5 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 3 | 0.5 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 3 | 0.5 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 3 | 0.5 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 3 | 0.5 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 4 | 0.5 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 4 | 0.5 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 4 | 0.5 |
| (1,1588) | 1:62:A:GLU:HA | 1:62:A:GLU:HG3 | 5 | 0.5 |
| (1,1569) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HB2 | 14 | 0.5 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 15 | 0.5 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 15 | 0.5 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 18 | 0.5 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 20 | 0.5 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 20 | 0.5 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 20 | 0.5 |
| (1,1485) | 1:28:A:PHE:HB2 | 1:95:A:VAL:HB | 15 | 0.5 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 10 | 0.5 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 10 | 0.5 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 10 | 0.5 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 17 | 0.5 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 3 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 3 | 0.5 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 3 | 0.5 |
| (1,1191) | 1:64:A:LEU:HD11 | 1:65:A:GLY:H | 14 | 0.5 |
| (1,1191) | 1:64:A:LEU:HD12 | 1:65:A:GLY:H | 14 | 0.5 |
| (1,1191) | 1:64:A:LEU:HD13 | 1:65:A:GLY:H | 14 | 0.5 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG11 | 18 | 0.5 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG12 | 18 | 0.5 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG13 | 18 | 0.5 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 14 | 0.5 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 13 | 0.5 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 13 | 0.5 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 13 | 0.5 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 10 | 0.5 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 10 | 0.5 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 10 | 0.5 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 16 | 0.5 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 16 | 0.5 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 16 | 0.5 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 9 | 0.5 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 20 | 0.5 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 20 | 0.5 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 20 | 0.5 |
| (1,326) | 1:184:A:LEU:HD11 | 1:187:A:LYS:H | 16 | 0.5 |
| (1,326) | 1:184:A:LEU:HD12 | 1:187:A:LYS:H | 16 | 0.5 |
| (1,326) | 1:184:A:LEU:HD13 | 1:187:A:LYS:H | 16 | 0.5 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 18 | 0.5 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 5 | 0.5 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 5 | 0.5 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 5 | 0.5 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 4 | 0.5 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 4 | 0.5 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 19 | 0.5 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 19 | 0.5 |
| (1,242) | 1:145:A:GLN:HE21 | 1:147:A:GLN:H | 19 | 0.5 |
| (1,128) | 1:12:A:LEU:HD11 | 1:159:A:GLN:H | 5 | 0.5 |
| (1,128) | 1:12:A:LEU:HD12 | 1:159:A:GLN:H | 5 | 0.5 |
| (1,128) | 1:12:A:LEU:HD13 | 1:159:A:GLN:H | 5 | 0.5 |
| (1,127) | 1:105:A:ALA:H | 1:107:A:ILE:HB | 4 | 0.5 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG11 | 11 | 0.5 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG12 | 11 | 0.5 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG13 | 11 | 0.5 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 13 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 15 | 0.5 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 12 | 0.49 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 12 | 0.49 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 12 | 0.49 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 12 | 0.49 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 12 | 0.49 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 12 | 0.49 |
| (1,3480) | 1:32:A:HIS:HD2 | 1:150:A:PRO:HG3 | 19 | 0.49 |
| (1,3420) | 1:60:A:HIS:HB3 | 1:75:A:TRP:HD1 | 10 | 0.49 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD1 | 19 | 0.49 |
| (1,3335) | 1:34:A:TYR:HB3 | 1:92:A:PHE:HD2 | 19 | 0.49 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB2 | 15 | 0.49 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB3 | 15 | 0.49 |
| (1,3277) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA3 | 1 | 0.49 |
| (1,3277) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA3 | 1 | 0.49 |
| (1,3277) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA3 | 1 | 0.49 |
| (1,3277) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA3 | 13 | 0.49 |
| (1,3277) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA3 | 13 | 0.49 |
| (1,3277) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA3 | 13 | 0.49 |
| (1,3276) | 1:118:A:GLY:HA3 | 1:121:A:TYR:HB3 | 1 | 0.49 |
| (1,3276) | 1:118:A:GLY:HA3 | 1:121:A:TYR:HB3 | 11 | 0.49 |
| (1,3276) | 1:118:A:GLY:HA3 | 1:121:A:TYR:HB3 | 14 | 0.49 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 2 | 0.49 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 2 | 0.49 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 2 | 0.49 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 2 | 0.49 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 2 | 0.49 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 2 | 0.49 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 6 | 0.49 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 6 | 0.49 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 6 | 0.49 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 18 | 0.49 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 18 | 0.49 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 18 | 0.49 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 19 | 0.49 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 19 | 0.49 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 19 | 0.49 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG11 | 20 | 0.49 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG12 | 20 | 0.49 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG13 | 20 | 0.49 |
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 17 | 0.49 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 15 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 15 | 0.49 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 15 | 0.49 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 8 | 0.49 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 8 | 0.49 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 8 | 0.49 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 17 | 0.49 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 17 | 0.49 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 17 | 0.49 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 17 | 0.49 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 17 | 0.49 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 17 | 0.49 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 17 | 0.49 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 17 | 0.49 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 17 | 0.49 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG11 | 11 | 0.49 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG12 | 11 | 0.49 |
| (1,2732) | 1:35:A:GLN:HA | 1:39:A:VAL:HG13 | 11 | 0.49 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 2 | 0.49 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 2 | 0.49 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 2 | 0.49 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 3 | 0.49 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 3 | 0.49 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 3 | 0.49 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 7 | 0.49 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 7 | 0.49 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 7 | 0.49 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 16 | 0.49 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 16 | 0.49 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 16 | 0.49 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 7 | 0.49 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 7 | 0.49 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 7 | 0.49 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 1 | 0.49 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 1 | 0.49 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 1 | 0.49 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 1 | 0.49 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 11 | 0.49 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 11 | 0.49 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 11 | 0.49 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 13 | 0.49 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 13 | 0.49 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 2 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 2 | 0.49 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 2 | 0.49 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 16 | 0.49 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 16 | 0.49 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 7 | 0.49 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 7 | 0.49 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 7 | 0.49 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 7 | 0.49 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 7 | 0.49 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 7 | 0.49 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG21 | 17 | 0.49 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG22 | 17 | 0.49 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG23 | 17 | 0.49 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG21 | 17 | 0.49 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG22 | 17 | 0.49 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG23 | 17 | 0.49 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG21 | 17 | 0.49 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG22 | 17 | 0.49 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG23 | 17 | 0.49 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 12 | 0.49 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 14 | 0.49 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 17 | 0.49 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 18 | 0.49 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 20 | 0.49 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 13 | 0.49 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 2 | 0.49 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 10 | 0.49 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 9 | 0.49 |
| (1,1931) | 1:62:A:GLU:HB2 | 1:63:A:PHE:HB3 | 16 | 0.49 |
| (1,1931) | 1:62:A:GLU:HB3 | 1:63:A:PHE:HB3 | 16 | 0.49 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 2 | 0.49 |
| (1,1624) | 1:33:A:CYS:HA | 1:150:A:PRO:HB2 | 19 | 0.49 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB2 | 16 | 0.49 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB3 | 16 | 0.49 |
| (1,1606) | 1:52:A:GLU:HG2 | 1:53:A:GLY:HA3 | 18 | 0.49 |
| (1,1606) | 1:52:A:GLU:HG3 | 1:53:A:GLY:HA3 | 18 | 0.49 |
| (1,1604) | 1:61:A:VAL:HA | 1:62:A:GLU:HG2 | 5 | 0.49 |
| (1,1588) | 1:62:A:GLU:HA | 1:62:A:GLU:HG3 | 6 | 0.49 |
| (1,1581) | 1:62:A:GLU:HA | 1:62:A:GLU:HG2 | 6 | 0.49 |
| (1,1581) | 1:62:A:GLU:HA | 1:62:A:GLU:HG2 | 14 | 0.49 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 15 | 0.49 |
| (1,1538) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB3 | 10 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1538) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB3 | 10 | 0.49 |
| (1,1538) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB3 | 10 | 0.49 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 10 | 0.49 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG11 | 6 | 0.49 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG12 | 6 | 0.49 |
| (1,1499) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HG13 | 6 | 0.49 |
| (1,1485) | 1:28:A:PHE:HB2 | 1:95:A:VAL:HB | 18 | 0.49 |
| (1,1430) | 1:117:A:LYS:H | 1:120:A:ASP:HB2 | 13 | 0.49 |
| (1,1409) | 1:67:A:LEU:HB2 | 1:70:A:ASP:HB3 | 15 | 0.49 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 4 | 0.49 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 4 | 0.49 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 4 | 0.49 |
| (1,1358) | 1:179:A:ASP:HB3 | 1:183:A:GLN:HE21 | 6 | 0.49 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE2 | 15 | 0.49 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE3 | 15 | 0.49 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE2 | 15 | 0.49 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE3 | 15 | 0.49 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE2 | 15 | 0.49 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE3 | 15 | 0.49 |
| (1,1331) | 1:70:A:ASP:HB3 | 1:72:A:THR:H | 12 | 0.49 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB2 | 2 | 0.49 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB3 | 2 | 0.49 |
| (1,1258) | 1:163:A:GLN:HG2 | 1:164:A:GLY:HA3 | 15 | 0.49 |
| (1,1258) | 1:163:A:GLN:HG3 | 1:164:A:GLY:HA3 | 15 | 0.49 |
| (1,1191) | 1:64:A:LEU:HD11 | 1:65:A:GLY:H | 1 | 0.49 |
| (1,1191) | 1:64:A:LEU:HD12 | 1:65:A:GLY:H | 1 | 0.49 |
| (1,1191) | 1:64:A:LEU:HD13 | 1:65:A:GLY:H | 1 | 0.49 |
| (1,1191) | 1:64:A:LEU:HD11 | 1:65:A:GLY:H | 17 | 0.49 |
| (1,1191) | 1:64:A:LEU:HD12 | 1:65:A:GLY:H | 17 | 0.49 |
| (1,1191) | 1:64:A:LEU:HD13 | 1:65:A:GLY:H | 17 | 0.49 |
| (1,1191) | 1:64:A:LEU:HD11 | 1:65:A:GLY:H | 18 | 0.49 |
| (1,1191) | 1:64:A:LEU:HD12 | 1:65:A:GLY:H | 18 | 0.49 |
| (1,1191) | 1:64:A:LEU:HD13 | 1:65:A:GLY:H | 18 | 0.49 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 8 | 0.49 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 8 | 0.49 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 8 | 0.49 |
| (1,778) | 1:51:A:PRO:HB3 | 1:54:A:THR:H | 1 | 0.49 |
| (1,765) | 1:106:A:ASP:H | 1:106:A:ASP:HB3 | 16 | 0.49 |
| (1,683) | 1:168:A:SER:H | 1:170:A:MET:HG2 | 1 | 0.49 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 4 | 0.49 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 13 | 0.49 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 13 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 13 | 0.49 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 5 | 0.49 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 14 | 0.49 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 14 | 0.49 |
| (1,163) | 1:69:A:LYS:H | 1:70:A:ASP:HB3 | 17 | 0.49 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 2 | 0.48 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 2 | 0.48 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 17 | 0.48 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 17 | 0.48 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 17 | 0.48 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 17 | 0.48 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 2 | 0.48 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 2 | 0.48 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 2 | 0.48 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 2 | 0.48 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 2 | 0.48 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 2 | 0.48 |
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 16 | 0.48 |
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 16 | 0.48 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB2 | 10 | 0.48 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB3 | 10 | 0.48 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB2 | 19 | 0.48 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB3 | 19 | 0.48 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 1 | 0.48 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 2 | 0.48 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 2 | 0.48 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 2 | 0.48 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 14 | 0.48 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 14 | 0.48 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 14 | 0.48 |
| (1,3230) | 1:87:A:ILE:HA | 1:90:A:PRO:HD3 | 8 | 0.48 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 1 | 0.48 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 1 | 0.48 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 1 | 0.48 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 2 | 0.48 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 2 | 0.48 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 2 | 0.48 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 5 | 0.48 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 5 | 0.48 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 5 | 0.48 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 11 | 0.48 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 11 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 11 | 0.48 |
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 16 | 0.48 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 16 | 0.48 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 16 | 0.48 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 3 | 0.48 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 3 | 0.48 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 3 | 0.48 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 4 | 0.48 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 4 | 0.48 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 4 | 0.48 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 1 | 0.48 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 1 | 0.48 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 1 | 0.48 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 9 | 0.48 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 9 | 0.48 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 9 | 0.48 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 13 | 0.48 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 13 | 0.48 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 13 | 0.48 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 18 | 0.48 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 18 | 0.48 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 18 | 0.48 |
| (1,2588) | 1:70:A:ASP:HA | 1:72:A:THR:H | 4 | 0.48 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 3 | 0.48 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 15 | 0.48 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 15 | 0.48 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 15 | 0.48 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 15 | 0.48 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 7 | 0.48 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 7 | 0.48 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 7 | 0.48 |
| (1,2452) | 1:149:A:VAL:HG11 | 1:150:A:PRO:HG3 | 10 | 0.48 |
| (1,2452) | 1:149:A:VAL:HG12 | 1:150:A:PRO:HG3 | 10 | 0.48 |
| (1,2452) | 1:149:A:VAL:HG13 | 1:150:A:PRO:HG3 | 10 | 0.48 |
| (1,2452) | 1:149:A:VAL:HG21 | 1:150:A:PRO:HG3 | 10 | 0.48 |
| (1,2452) | 1:149:A:VAL:HG22 | 1:150:A:PRO:HG3 | 10 | 0.48 |
| (1,2452) | 1:149:A:VAL:HG23 | 1:150:A:PRO:HG3 | 10 | 0.48 |
| (1,2452) | 1:149:A:VAL:HG11 | 1:150:A:PRO:HG3 | 12 | 0.48 |
| (1,2452) | 1:149:A:VAL:HG12 | 1:150:A:PRO:HG3 | 12 | 0.48 |
| (1,2452) | 1:149:A:VAL:HG13 | 1:150:A:PRO:HG3 | 12 | 0.48 |
| (1,2452) | 1:149:A:VAL:HG21 | 1:150:A:PRO:HG3 | 12 | 0.48 |
| (1,2452) | 1:149:A:VAL:HG22 | 1:150:A:PRO:HG3 | 12 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2452) | 1:149:A:VAL:HG23 | 1:150:A:PRO:HG3 | 12 | 0.48 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 4 | 0.48 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 13 | 0.48 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 19 | 0.48 |
| (1,2316) | 1:117:A:LYS:H | 1:117:A:LYS:HG2 | 10 | 0.48 |
| (1,2291) | 1:117:A:LYS:HG3 | 1:120:A:ASP:H | 20 | 0.48 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 6 | 0.48 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 6 | 0.48 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 6 | 0.48 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 6 | 0.48 |
| (1,2168) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HG2 | 2 | 0.48 |
| (1,2168) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HG2 | 2 | 0.48 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG21 | 20 | 0.48 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG22 | 20 | 0.48 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG23 | 20 | 0.48 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG21 | 20 | 0.48 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG22 | 20 | 0.48 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG23 | 20 | 0.48 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG21 | 20 | 0.48 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG22 | 20 | 0.48 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG23 | 20 | 0.48 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 16 | 0.48 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 16 | 0.48 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 16 | 0.48 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB2 | 13 | 0.48 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB3 | 13 | 0.48 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 4 | 0.48 |
| (1,2016) | 1:117:A:LYS:HD3 | 1:119:A:GLU:H | 2 | 0.48 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 2 | 0.48 |
| (1,1867) | 1:37:A:GLU:HB2 | 1:38:A:GLU:HA | 18 | 0.48 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 18 | 0.48 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD1 | 15 | 0.48 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD2 | 15 | 0.48 |
| (1,1624) | 1:33:A:CYS:HA | 1:150:A:PRO:HB2 | 15 | 0.48 |
| (1,1603) | 1:62:A:GLU:HG2 | 1:63:A:PHE:H | 20 | 0.48 |
| (1,1588) | 1:62:A:GLU:HA | 1:62:A:GLU:HG3 | 8 | 0.48 |
| (1,1588) | 1:62:A:GLU:HA | 1:62:A:GLU:HG3 | 20 | 0.48 |
| (1,1581) | 1:62:A:GLU:HA | 1:62:A:GLU:HG2 | 10 | 0.48 |
| (1,1581) | 1:62:A:GLU:HA | 1:62:A:GLU:HG2 | 12 | 0.48 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 15 | 0.48 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 15 | 0.48 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 15 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 7 | 0.48 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 7 | 0.48 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 20 | 0.48 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 20 | 0.48 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 20 | 0.48 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 20 | 0.48 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 20 | 0.48 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG11 | 16 | 0.48 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG12 | 16 | 0.48 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG13 | 16 | 0.48 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 5 | 0.48 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 5 | 0.48 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 5 | 0.48 |
| (1,1409) | 1:67:A:LEU:HB2 | 1:70:A:ASP:HB3 | 12 | 0.48 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB2 | 10 | 0.48 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB3 | 10 | 0.48 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 15 | 0.48 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 15 | 0.48 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 15 | 0.48 |
| (1,1298) | 1:141:A:ALA:HA | 1:146:A:LEU:HB2 | 5 | 0.48 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 3 | 0.48 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 12 | 0.48 |
| (1,1213) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE21 | 7 | 0.48 |
| (1,1213) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE21 | 7 | 0.48 |
| (1,1213) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE21 | 7 | 0.48 |
| (1,1191) | 1:64:A:LEU:HD11 | 1:65:A:GLY:H | 10 | 0.48 |
| (1,1191) | 1:64:A:LEU:HD12 | 1:65:A:GLY:H | 10 | 0.48 |
| (1,1191) | 1:64:A:LEU:HD13 | 1:65:A:GLY:H | 10 | 0.48 |
| (1,1080) | 1:34:A:TYR:HD1 | 1:38:A:GLU:H | 5 | 0.48 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 18 | 0.48 |
| (1,1012) | 1:169:A:ASN:HB3 | 1:169:A:ASN:HD22 | 1 | 0.48 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG21 | 10 | 0.48 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG22 | 10 | 0.48 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG23 | 10 | 0.48 |
| (1,929) | 1:183:A:GLN:H | 1:183:A:GLN:HB3 | 16 | 0.48 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 6 | 0.48 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 15 | 0.48 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 6 | 0.48 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 6 | 0.48 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 6 | 0.48 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 11 | 0.48 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 11 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 11 | 0.48 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD21 | 15 | 0.48 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD22 | 15 | 0.48 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD23 | 15 | 0.48 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 3 | 0.48 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 3 | 0.48 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 3 | 0.48 |
| (1,765) | 1:106:A:ASP:H | 1:106:A:ASP:HB3 | 4 | 0.48 |
| (1,765) | 1:106:A:ASP:H | 1:106:A:ASP:HB3 | 20 | 0.48 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 19 | 0.48 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 19 | 0.48 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 19 | 0.48 |
| (1,401) | 1:117:A:LYS:HB2 | 1:120:A:ASP:H | 18 | 0.48 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 1 | 0.48 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 1 | 0.48 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 1 | 0.48 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 19 | 0.48 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 19 | 0.48 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 19 | 0.48 |
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 12 | 0.48 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 8 | 0.48 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 8 | 0.48 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 8 | 0.48 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 6 | 0.48 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 6 | 0.48 |
| (1,132) | 1:56:A:MET:HB2 | 1:57:A:THR:H | 10 | 0.48 |
| (1,132) | 1:56:A:MET:HB2 | 1:57:A:THR:H | 19 | 0.48 |
| (1,111) | 1:103:A:SER:HB2 | 1:105:A:ALA:H | 19 | 0.48 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG11 | 8 | 0.48 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG12 | 8 | 0.48 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG13 | 8 | 0.48 |
| (1,67) | 1:26:A:PHE:H | 1:59:A:TYR:H | 15 | 0.48 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 14 | 0.47 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 14 | 0.47 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE1 | 18 | 0.47 |
| (1,3515) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HE2 | 18 | 0.47 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB2 | 18 | 0.47 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB3 | 18 | 0.47 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB2 | 18 | 0.47 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB3 | 18 | 0.47 |
| (1,3481) | 1:29:A:TYR:HE1 | 1:67:A:LEU:HA | 19 | 0.47 |
| (1,3481) | 1:29:A:TYR:HE2 | 1:67:A:LEU:HA | 19 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3297) | 1:23:A:LEU:HB2 | 1:153:A:TYR:H | 13 | 0.47 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 10 | 0.47 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 13 | 0.47 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 13 | 0.47 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 13 | 0.47 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 15 | 0.47 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 15 | 0.47 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 15 | 0.47 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG21 | 2 | 0.47 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG22 | 2 | 0.47 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG23 | 2 | 0.47 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG21 | 2 | 0.47 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG22 | 2 | 0.47 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG23 | 2 | 0.47 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG21 | 2 | 0.47 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG22 | 2 | 0.47 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG23 | 2 | 0.47 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG21 | 2 | 0.47 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG22 | 2 | 0.47 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG23 | 2 | 0.47 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG21 | 2 | 0.47 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG22 | 2 | 0.47 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG23 | 2 | 0.47 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG21 | 2 | 0.47 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG22 | 2 | 0.47 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG23 | 2 | 0.47 |
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 20 | 0.47 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 20 | 0.47 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 20 | 0.47 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 8 | 0.47 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 4 | 0.47 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 4 | 0.47 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 4 | 0.47 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD11 | 10 | 0.47 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD12 | 10 | 0.47 |
| (1,2861) | 1:12:A:LEU:HA | 1:12:A:LEU:HD13 | 10 | 0.47 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 14 | 0.47 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 14 | 0.47 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 14 | 0.47 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 15 | 0.47 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 15 | 0.47 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 15 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 8 | 0.47 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 8 | 0.47 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 8 | 0.47 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 8 | 0.47 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 8 | 0.47 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 8 | 0.47 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 8 | 0.47 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 8 | 0.47 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 8 | 0.47 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 7 | 0.47 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 19 | 0.47 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 3 | 0.47 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 3 | 0.47 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 3 | 0.47 |
| (1,2474) | 1:83:A:VAL:HA | 1:84:A:GLU:HB2 | 16 | 0.47 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG11 | 1 | 0.47 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG12 | 1 | 0.47 |
| (1,2471) | 1:46:A:VAL:H | 1:46:A:VAL:HG13 | 1 | 0.47 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE1 | 11 | 0.47 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE2 | 11 | 0.47 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE1 | 11 | 0.47 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE2 | 11 | 0.47 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE1 | 11 | 0.47 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE2 | 11 | 0.47 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 5 | 0.47 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 5 | 0.47 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 5 | 0.47 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 16 | 0.47 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 16 | 0.47 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 16 | 0.47 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 20 | 0.47 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 20 | 0.47 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 20 | 0.47 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 20 | 0.47 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 20 | 0.47 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 20 | 0.47 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 3 | 0.47 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 19 | 0.47 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 19 | 0.47 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 19 | 0.47 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 19 | 0.47 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 19 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 19 | 0.47 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG21 | 16 | 0.47 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG22 | 16 | 0.47 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG23 | 16 | 0.47 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG21 | 16 | 0.47 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG22 | 16 | 0.47 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG23 | 16 | 0.47 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG21 | 16 | 0.47 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG22 | 16 | 0.47 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG23 | 16 | 0.47 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 9 | 0.47 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 15 | 0.47 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 1 | 0.47 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 15 | 0.47 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 1 | 0.47 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 11 | 0.47 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 7 | 0.47 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 7 | 0.47 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 7 | 0.47 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 14 | 0.47 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 14 | 0.47 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 14 | 0.47 |
| (1,1878) | 1:60:A:HIS:HB2 | 1:72:A:THR:HG21 | 6 | 0.47 |
| (1,1878) | 1:60:A:HIS:HB2 | 1:72:A:THR:HG22 | 6 | 0.47 |
| (1,1878) | 1:60:A:HIS:HB2 | 1:72:A:THR:HG23 | 6 | 0.47 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 4 | 0.47 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 9 | 0.47 |
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 6 | 0.47 |
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 9 | 0.47 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 9 | 0.47 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 9 | 0.47 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 9 | 0.47 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 17 | 0.47 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB2 | 4 | 0.47 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB3 | 4 | 0.47 |
| (1,1604) | 1:61:A:VAL:HA | 1:62:A:GLU:HG2 | 16 | 0.47 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 13 | 0.47 |
| (1,1588) | 1:62:A:GLU:HA | 1:62:A:GLU:HG3 | 1 | 0.47 |
| (1,1588) | 1:62:A:GLU:HA | 1:62:A:GLU:HG3 | 10 | 0.47 |
| (1,1581) | 1:62:A:GLU:HA | 1:62:A:GLU:HG2 | 5 | 0.47 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 12 | 0.47 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 5 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 5 | 0.47 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 5 | 0.47 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 6 | 0.47 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 6 | 0.47 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 6 | 0.47 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG11 | 2 | 0.47 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG12 | 2 | 0.47 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG13 | 2 | 0.47 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 7 | 0.47 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 7 | 0.47 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 7 | 0.47 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 7 | 0.47 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 7 | 0.47 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 7 | 0.47 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 13 | 0.47 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 13 | 0.47 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 13 | 0.47 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE2 | 8 | 0.47 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE3 | 8 | 0.47 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE2 | 8 | 0.47 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE3 | 8 | 0.47 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE2 | 8 | 0.47 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE3 | 8 | 0.47 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 9 | 0.47 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 9 | 0.47 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 9 | 0.47 |
| (1,1331) | 1:70:A:ASP:HB3 | 1:72:A:THR:H | 3 | 0.47 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 16 | 0.47 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 18 | 0.47 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 18 | 0.47 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 18 | 0.47 |
| (1,1213) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE21 | 10 | 0.47 |
| (1,1213) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE21 | 10 | 0.47 |
| (1,1213) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE21 | 10 | 0.47 |
| (1,1084) | 1:37:A:GLU:HG3 | 1:38:A:GLU:H | 4 | 0.47 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 10 | 0.47 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 11 | 0.47 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 16 | 0.47 |
| (1,765) | 1:106:A:ASP:H | 1:106:A:ASP:HB3 | 11 | 0.47 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 2 | 0.47 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 8 | 0.47 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 8 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 8 | 0.47 |
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 10 | 0.47 |
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 13 | 0.47 |
| (1,606) | 1:137:A:GLN:H | 1:137:A:GLN:HG2 | 2 | 0.47 |
| (1,606) | 1:137:A:GLN:H | 1:137:A:GLN:HG2 | 12 | 0.47 |
| (1,606) | 1:137:A:GLN:H | 1:137:A:GLN:HG2 | 19 | 0.47 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 13 | 0.47 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 13 | 0.47 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 13 | 0.47 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 16 | 0.47 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 16 | 0.47 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 16 | 0.47 |
| (1,587) | 1:46:A:VAL:HG21 | 1:47:A:ARG:H | 10 | 0.47 |
| (1,587) | 1:46:A:VAL:HG22 | 1:47:A:ARG:H | 10 | 0.47 |
| (1,587) | 1:46:A:VAL:HG23 | 1:47:A:ARG:H | 10 | 0.47 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 19 | 0.47 |
| (1,498) | 1:77:A:VAL:HG11 | 1:124:A:ALA:H | 9 | 0.47 |
| (1,498) | 1:77:A:VAL:HG12 | 1:124:A:ALA:H | 9 | 0.47 |
| (1,498) | 1:77:A:VAL:HG13 | 1:124:A:ALA:H | 9 | 0.47 |
| (1,441) | 1:34:A:TYR:HE2 | 1:92:A:PHE:H | 6 | 0.47 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 16 | 0.47 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 16 | 0.47 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 16 | 0.47 |
| (1,285) | 1:152:A:MET:H | 1:152:A:MET:HB3 | 12 | 0.47 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 3 | 0.47 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 3 | 0.47 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 3 | 0.47 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 8 | 0.47 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 8 | 0.47 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 10 | 0.47 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 10 | 0.47 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 15 | 0.47 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 15 | 0.47 |
| (1,160) | 1:67:A:LEU:HD11 | 1:69:A:LYS:H | 18 | 0.47 |
| (1,160) | 1:67:A:LEU:HD12 | 1:69:A:LYS:H | 18 | 0.47 |
| (1,160) | 1:67:A:LEU:HD13 | 1:69:A:LYS:H | 18 | 0.47 |
| (1,112) | 1:105:A:ALA:H | 1:106:A:ASP:HB3 | 7 | 0.47 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 9 | 0.46 |
| (1,3355) | 1:25:A:PHE:HD1 | 1:146:A:LEU:HD11 | 11 | 0.46 |
| (1,3355) | 1:25:A:PHE:HD1 | 1:146:A:LEU:HD12 | 11 | 0.46 |
| (1,3355) | 1:25:A:PHE:HD1 | 1:146:A:LEU:HD13 | 11 | 0.46 |
| (1,3355) | 1:25:A:PHE:HD2 | 1:146:A:LEU:HD11 | 11 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3355) | 1:25:A:PHE:HD2 | 1:146:A:LEU:HD12 | 11 | 0.46 |
| (1,3355) | 1:25:A:PHE:HD2 | 1:146:A:LEU:HD13 | 11 | 0.46 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD1 | 8 | 0.46 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD2 | 8 | 0.46 |
| (1,3311) | 1:29:A:TYR:HD1 | 1:71:A:LEU:HB2 | 1 | 0.46 |
| (1,3311) | 1:29:A:TYR:HD2 | 1:71:A:LEU:HB2 | 1 | 0.46 |
| (1,3274) | 1:118:A:GLY:HA3 | 1:121:A:TYR:H | 1 | 0.46 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 4 | 0.46 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 4 | 0.46 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 4 | 0.46 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 20 | 0.46 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 20 | 0.46 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 20 | 0.46 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG11 | 7 | 0.46 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG12 | 7 | 0.46 |
| (1,2730) | 1:39:A:VAL:H | 1:39:A:VAL:HG13 | 7 | 0.46 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 4 | 0.46 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 4 | 0.46 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 4 | 0.46 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG21 | 8 | 0.46 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG22 | 8 | 0.46 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG23 | 8 | 0.46 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG21 | 8 | 0.46 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG22 | 8 | 0.46 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG23 | 8 | 0.46 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG21 | 8 | 0.46 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG22 | 8 | 0.46 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG23 | 8 | 0.46 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG21 | 7 | 0.46 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG22 | 7 | 0.46 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG23 | 7 | 0.46 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG21 | 7 | 0.46 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG22 | 7 | 0.46 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG23 | 7 | 0.46 |
| (1,2588) | 1:70:A:ASP:HA | 1:72:A:THR:H | 6 | 0.46 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 1 | 0.46 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 1 | 0.46 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 1 | 0.46 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 16 | 0.46 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 19 | 0.46 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 2 | 0.46 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 2 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 2 | 0.46 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 3 | 0.46 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 3 | 0.46 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 3 | 0.46 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 10 | 0.46 |
| (1,2316) | 1:117:A:LYS:H | 1:117:A:LYS:HG2 | 2 | 0.46 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 15 | 0.46 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 15 | 0.46 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 15 | 0.46 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 11 | 0.46 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 11 | 0.46 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 11 | 0.46 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 11 | 0.46 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 11 | 0.46 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 11 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG21 | 1 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG22 | 1 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG23 | 1 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG21 | 1 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG22 | 1 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG23 | 1 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG21 | 1 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG22 | 1 | 0.46 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG23 | 1 | 0.46 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 3 | 0.46 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 3 | 0.46 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 3 | 0.46 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 7 | 0.46 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 10 | 0.46 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 12 | 0.46 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 19 | 0.46 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 15 | 0.46 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 4 | 0.46 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 9 | 0.46 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 16 | 0.46 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 17 | 0.46 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB2 | 1 | 0.46 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB3 | 1 | 0.46 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB2 | 1 | 0.46 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB3 | 1 | 0.46 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB2 | 1 | 0.46 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB3 | 1 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 1 | 0.46 |
| (1,1686) | 1:99:A:GLN:HG3 | 1:100:A:THR:H | 4 | 0.46 |
| (1,1669) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HG2 | 5 | 0.46 |
| (1,1669) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HG2 | 5 | 0.46 |
| (1,1669) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HG2 | 5 | 0.46 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB2 | 13 | 0.46 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB3 | 13 | 0.46 |
| (1,1603) | 1:62:A:GLU:HG2 | 1:63:A:PHE:H | 17 | 0.46 |
| (1,1581) | 1:62:A:GLU:HA | 1:62:A:GLU:HG2 | 7 | 0.46 |
| (1,1581) | 1:62:A:GLU:HA | 1:62:A:GLU:HG2 | 20 | 0.46 |
| (1,1547) | 1:152:A:MET:HB3 | 1:160:A:LEU:HD11 | 17 | 0.46 |
| (1,1547) | 1:152:A:MET:HB3 | 1:160:A:LEU:HD12 | 17 | 0.46 |
| (1,1547) | 1:152:A:MET:HB3 | 1:160:A:LEU:HD13 | 17 | 0.46 |
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 9 | 0.46 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 9 | 0.46 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 9 | 0.46 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 5 | 0.46 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 7 | 0.46 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 5 | 0.46 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 5 | 0.46 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 5 | 0.46 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG11 | 1 | 0.46 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG12 | 1 | 0.46 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG13 | 1 | 0.46 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 19 | 0.46 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 19 | 0.46 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 19 | 0.46 |
| (1,1409) | 1:67:A:LEU:HB2 | 1:70:A:ASP:HB3 | 5 | 0.46 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 19 | 0.46 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB2 | 8 | 0.46 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB3 | 8 | 0.46 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 18 | 0.46 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 18 | 0.46 |
| (1,911) | 1:127:A:SER:H | 1:131:A:LYS:HD3 | 15 | 0.46 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 15 | 0.46 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 7 | 0.46 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 12 | 0.46 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 12 | 0.46 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 12 | 0.46 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 12 | 0.46 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 15 | 0.46 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 15 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 15 | 0.46 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 2 | 0.46 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 2 | 0.46 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 2 | 0.46 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 1 | 0.46 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 11 | 0.46 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 9 | 0.46 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 9 | 0.46 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 9 | 0.46 |
| (1,765) | 1:106:A:ASP:H | 1:106:A:ASP:HB3 | 19 | 0.46 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 6 | 0.46 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 6 | 0.46 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 6 | 0.46 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 13 | 0.46 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 13 | 0.46 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 13 | 0.46 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 8 | 0.46 |
| (1,560) | 1:42:A:VAL:HG21 | 1:178:A:ALA:H | 15 | 0.46 |
| (1,560) | 1:42:A:VAL:HG22 | 1:178:A:ALA:H | 15 | 0.46 |
| (1,560) | 1:42:A:VAL:HG23 | 1:178:A:ALA:H | 15 | 0.46 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 14 | 0.46 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 14 | 0.46 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 14 | 0.46 |
| (1,438) | 1:60:A:HIS:HB2 | 1:75:A:TRP:H | 9 | 0.46 |
| (1,285) | 1:152:A:MET:H | 1:152:A:MET:HB3 | 1 | 0.46 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 2 | 0.46 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 2 | 0.46 |
| (1,132) | 1:56:A:MET:HB2 | 1:57:A:THR:H | 5 | 0.46 |
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 2 | 0.46 |
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 17 | 0.46 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE1 | 16 | 0.45 |
| (1,3517) | 1:42:A:VAL:HG21 | 1:177:A:TYR:HE2 | 16 | 0.45 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE1 | 16 | 0.45 |
| (1,3517) | 1:42:A:VAL:HG22 | 1:177:A:TYR:HE2 | 16 | 0.45 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE1 | 16 | 0.45 |
| (1,3517) | 1:42:A:VAL:HG23 | 1:177:A:TYR:HE2 | 16 | 0.45 |
| (1,3421) | 1:59:A:TYR:HB2 | 1:75:A:TRP:HD1 | 14 | 0.45 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE1 | 10 | 0.45 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE2 | 10 | 0.45 |
| (1,3297) | 1:23:A:LEU:HB2 | 1:153:A:TYR:H | 19 | 0.45 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 18 | 0.45 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 18 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 18 | 0.45 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 4 | 0.45 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 4 | 0.45 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 4 | 0.45 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 4 | 0.45 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 4 | 0.45 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 4 | 0.45 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 4 | 0.45 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 4 | 0.45 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 4 | 0.45 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 7 | 0.45 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 7 | 0.45 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 7 | 0.45 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 9 | 0.45 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 9 | 0.45 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 9 | 0.45 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB1 | 10 | 0.45 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB2 | 10 | 0.45 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB3 | 10 | 0.45 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB1 | 10 | 0.45 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB2 | 10 | 0.45 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB3 | 10 | 0.45 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB1 | 10 | 0.45 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB2 | 10 | 0.45 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB3 | 10 | 0.45 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG11 | 17 | 0.45 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG12 | 17 | 0.45 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG13 | 17 | 0.45 |
| (1,2943) | 1:3:A:ILE:HG21 | 1:8:A:GLN:HG3 | 16 | 0.45 |
| (1,2943) | 1:3:A:ILE:HG22 | 1:8:A:GLN:HG3 | 16 | 0.45 |
| (1,2943) | 1:3:A:ILE:HG23 | 1:8:A:GLN:HG3 | 16 | 0.45 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 10 | 0.45 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 10 | 0.45 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 10 | 0.45 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 6 | 0.45 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 6 | 0.45 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 6 | 0.45 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 6 | 0.45 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 6 | 0.45 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 6 | 0.45 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 6 | 0.45 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG21 | 8 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG22 | 8 | 0.45 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG23 | 8 | 0.45 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG21 | 8 | 0.45 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG22 | 8 | 0.45 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG23 | 8 | 0.45 |
| (1,2588) | 1:70:A:ASP:HA | 1:72:A:THR:H | 12 | 0.45 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 9 | 0.45 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 9 | 0.45 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 9 | 0.45 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 5 | 0.45 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 5 | 0.45 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 5 | 0.45 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 5 | 0.45 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 5 | 0.45 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 5 | 0.45 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 5 | 0.45 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 5 | 0.45 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 5 | 0.45 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 8 | 0.45 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 8 | 0.45 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 8 | 0.45 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 8 | 0.45 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 8 | 0.45 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 8 | 0.45 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 3 | 0.45 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 3 | 0.45 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 3 | 0.45 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 1 | 0.45 |
| (1,2382) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HG2 | 7 | 0.45 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 9 | 0.45 |
| (1,2371) | 1:157:A:LYS:HA | 1:157:A:LYS:HG2 | 9 | 0.45 |
| (1,2291) | 1:117:A:LYS:HG3 | 1:120:A:ASP:H | 2 | 0.45 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 8 | 0.45 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 8 | 0.45 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 8 | 0.45 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 12 | 0.45 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 5 | 0.45 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 5 | 0.45 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 5 | 0.45 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 10 | 0.45 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 10 | 0.45 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 10 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 10 | 0.45 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 10 | 0.45 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 10 | 0.45 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG21 | 11 | 0.45 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG22 | 11 | 0.45 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG23 | 11 | 0.45 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG21 | 11 | 0.45 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG22 | 11 | 0.45 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG23 | 11 | 0.45 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG21 | 11 | 0.45 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG22 | 11 | 0.45 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG23 | 11 | 0.45 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 5 | 0.45 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 6 | 0.45 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 12 | 0.45 |
| (1,1931) | 1:62:A:GLU:HB2 | 1:63:A:PHE:HB3 | 10 | 0.45 |
| (1,1931) | 1:62:A:GLU:HB3 | 1:63:A:PHE:HB3 | 10 | 0.45 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB2 | 4 | 0.45 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB3 | 4 | 0.45 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB2 | 4 | 0.45 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB3 | 4 | 0.45 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB2 | 4 | 0.45 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB3 | 4 | 0.45 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 18 | 0.45 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 18 | 0.45 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 18 | 0.45 |
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 15 | 0.45 |
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 15 | 0.45 |
| (1,1686) | 1:99:A:GLN:HG3 | 1:100:A:THR:H | 2 | 0.45 |
| (1,1686) | 1:99:A:GLN:HG3 | 1:100:A:THR:H | 8 | 0.45 |
| (1,1669) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HG2 | 12 | 0.45 |
| (1,1669) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HG2 | 12 | 0.45 |
| (1,1669) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HG2 | 12 | 0.45 |
| (1,1632) | 1:31:A:PRO:HA | 1:96:A:GLN:HG2 | 18 | 0.45 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 2 | 0.45 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 2 | 0.45 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 16 | 0.45 |
| (1,1588) | 1:62:A:GLU:HA | 1:62:A:GLU:HG3 | 12 | 0.45 |
| (1,1581) | 1:62:A:GLU:HA | 1:62:A:GLU:HG2 | 2 | 0.45 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 8 | 0.45 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 8 | 0.45 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 8 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 20 | 0.45 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 20 | 0.45 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 20 | 0.45 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 1 | 0.45 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 1 | 0.45 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 3 | 0.45 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 3 | 0.45 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 13 | 0.45 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 13 | 0.45 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 9 | 0.45 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 9 | 0.45 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 9 | 0.45 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 12 | 0.45 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 12 | 0.45 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 12 | 0.45 |
| (1,1366) | 1:34:A:TYR:HE1 | 1:97:A:LYS:HE3 | 1 | 0.45 |
| (1,1366) | 1:34:A:TYR:HE2 | 1:97:A:LYS:HE3 | 1 | 0.45 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 19 | 0.45 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 19 | 0.45 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 19 | 0.45 |
| (1,1258) | 1:163:A:GLN:HG2 | 1:164:A:GLY:HA3 | 4 | 0.45 |
| (1,1258) | 1:163:A:GLN:HG3 | 1:164:A:GLY:HA3 | 4 | 0.45 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 7 | 0.45 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 15 | 0.45 |
| (1,991) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HD22 | 14 | 0.45 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 12 | 0.45 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 16 | 0.45 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 16 | 0.45 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 16 | 0.45 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 4 | 0.45 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 4 | 0.45 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 4 | 0.45 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 16 | 0.45 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 16 | 0.45 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 16 | 0.45 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 13 | 0.45 |
| (1,765) | 1:106:A:ASP:H | 1:106:A:ASP:HB3 | 1 | 0.45 |
| (1,765) | 1:106:A:ASP:H | 1:106:A:ASP:HB3 | 6 | 0.45 |
| (1,765) | 1:106:A:ASP:H | 1:106:A:ASP:HB3 | 18 | 0.45 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 14 | 0.45 |
| (1,578) | 1:122:A:ASP:H | 1:122:A:ASP:HB3 | 7 | 0.45 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG11 | 7 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG12 | 7 | 0.45 |
| (1,541) | 1:181:A:VAL:H | 1:181:A:VAL:HG13 | 7 | 0.45 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 8 | 0.45 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 8 | 0.45 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 8 | 0.45 |
| (1,485) | 1:4:A:THR:H | 1:7:A:LYS:HB2 | 18 | 0.45 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 7 | 0.45 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 7 | 0.45 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 7 | 0.45 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 2 | 0.45 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 2 | 0.45 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 2 | 0.45 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 4 | 0.45 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 4 | 0.45 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 4 | 0.45 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 17 | 0.45 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 17 | 0.45 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 17 | 0.45 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG11 | 14 | 0.45 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG12 | 14 | 0.45 |
| (1,257) | 1:172:A:VAL:H | 1:172:A:VAL:HG13 | 14 | 0.45 |
| (1,132) | 1:56:A:MET:HB2 | 1:57:A:THR:H | 2 | 0.45 |
| (1,127) | 1:105:A:ALA:H | 1:107:A:ILE:HB | 20 | 0.45 |
| (1,111) | 1:103:A:SER:HB2 | 1:105:A:ALA:H | 11 | 0.45 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 5 | 0.44 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 5 | 0.44 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 5 | 0.44 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 5 | 0.44 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 5 | 0.44 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 5 | 0.44 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 4 | 0.44 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 4 | 0.44 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 7 | 0.44 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 7 | 0.44 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 7 | 0.44 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 12 | 0.44 |
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 20 | 0.44 |
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 20 | 0.44 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 20 | 0.44 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 20 | 0.44 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 20 | 0.44 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD11 | 8 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD12 | 8 | 0.44 |
| (1,3121) | 1:50:A:LEU:HA | 1:50:A:LEU:HD13 | 8 | 0.44 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB1 | 8 | 0.44 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB2 | 8 | 0.44 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB3 | 8 | 0.44 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 8 | 0.44 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 8 | 0.44 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 8 | 0.44 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG11 | 8 | 0.44 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG12 | 8 | 0.44 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG13 | 8 | 0.44 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG11 | 8 | 0.44 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG12 | 8 | 0.44 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG13 | 8 | 0.44 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG11 | 8 | 0.44 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG12 | 8 | 0.44 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG13 | 8 | 0.44 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 19 | 0.44 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 19 | 0.44 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 19 | 0.44 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 3 | 0.44 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 3 | 0.44 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 3 | 0.44 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 9 | 0.44 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 9 | 0.44 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 9 | 0.44 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 9 | 0.44 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 9 | 0.44 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 9 | 0.44 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 9 | 0.44 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 9 | 0.44 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 9 | 0.44 |
| (1,2588) | 1:70:A:ASP:HA | 1:72:A:THR:H | 2 | 0.44 |
| (1,2588) | 1:70:A:ASP:HA | 1:72:A:THR:H | 10 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 6 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 6 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 6 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 6 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 6 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 6 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 6 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 6 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 6 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 20 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 20 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 20 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 20 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 20 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 20 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 20 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 20 | 0.44 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 20 | 0.44 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 6 | 0.44 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 6 | 0.44 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 6 | 0.44 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 6 | 0.44 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 6 | 0.44 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 6 | 0.44 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 6 | 0.44 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 6 | 0.44 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 6 | 0.44 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 8 | 0.44 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 18 | 0.44 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 18 | 0.44 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 18 | 0.44 |
| (1,2452) | 1:149:A:VAL:HG11 | 1:150:A:PRO:HG3 | 9 | 0.44 |
| (1,2452) | 1:149:A:VAL:HG12 | 1:150:A:PRO:HG3 | 9 | 0.44 |
| (1,2452) | 1:149:A:VAL:HG13 | 1:150:A:PRO:HG3 | 9 | 0.44 |
| (1,2452) | 1:149:A:VAL:HG21 | 1:150:A:PRO:HG3 | 9 | 0.44 |
| (1,2452) | 1:149:A:VAL:HG22 | 1:150:A:PRO:HG3 | 9 | 0.44 |
| (1,2452) | 1:149:A:VAL:HG23 | 1:150:A:PRO:HG3 | 9 | 0.44 |
| (1,2291) | 1:117:A:LYS:HG3 | 1:120:A:ASP:H | 8 | 0.44 |
| (1,2291) | 1:117:A:LYS:HG3 | 1:120:A:ASP:H | 17 | 0.44 |
| (1,2195) | 1:66:A:PRO:HD2 | 1:67:A:LEU:HG | 8 | 0.44 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 8 | 0.44 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 8 | 0.44 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG11 | 7 | 0.44 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG12 | 7 | 0.44 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG13 | 7 | 0.44 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 10 | 0.44 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 8 | 0.44 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 9 | 0.44 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 6 | 0.44 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 19 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB2 | 13 | 0.44 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB3 | 13 | 0.44 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB2 | 13 | 0.44 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB3 | 13 | 0.44 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB2 | 13 | 0.44 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB3 | 13 | 0.44 |
| (1,1843) | 1:60:A:HIS:HB2 | 1:72:A:THR:HA | 2 | 0.44 |
| (1,1793) | 1:50:A:LEU:HD21 | 1:56:A:MET:HG3 | 20 | 0.44 |
| (1,1793) | 1:50:A:LEU:HD22 | 1:56:A:MET:HG3 | 20 | 0.44 |
| (1,1793) | 1:50:A:LEU:HD23 | 1:56:A:MET:HG3 | 20 | 0.44 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG2 | 1 | 0.44 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG3 | 1 | 0.44 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 18 | 0.44 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB2 | 8 | 0.44 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB3 | 8 | 0.44 |
| (1,1604) | 1:61:A:VAL:HA | 1:62:A:GLU:HG2 | 6 | 0.44 |
| (1,1581) | 1:62:A:GLU:HA | 1:62:A:GLU:HG2 | 4 | 0.44 |
| (1,1581) | 1:62:A:GLU:HA | 1:62:A:GLU:HG2 | 8 | 0.44 |
| (1,1581) | 1:62:A:GLU:HA | 1:62:A:GLU:HG2 | 9 | 0.44 |
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 6 | 0.44 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 6 | 0.44 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 6 | 0.44 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 2 | 0.44 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 2 | 0.44 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 3 | 0.44 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 1 | 0.44 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 1 | 0.44 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 1 | 0.44 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 3 | 0.44 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 2 | 0.44 |
| (1,1215) | 1:73:A:GLN:HE21 | 1:77:A:VAL:HG21 | 16 | 0.44 |
| (1,1215) | 1:73:A:GLN:HE21 | 1:77:A:VAL:HG22 | 16 | 0.44 |
| (1,1215) | 1:73:A:GLN:HE21 | 1:77:A:VAL:HG23 | 16 | 0.44 |
| (1,1191) | 1:64:A:LEU:HD11 | 1:65:A:GLY:H | 8 | 0.44 |
| (1,1191) | 1:64:A:LEU:HD12 | 1:65:A:GLY:H | 8 | 0.44 |
| (1,1191) | 1:64:A:LEU:HD13 | 1:65:A:GLY:H | 8 | 0.44 |
| (1,1191) | 1:64:A:LEU:HD11 | 1:65:A:GLY:H | 12 | 0.44 |
| (1,1191) | 1:64:A:LEU:HD12 | 1:65:A:GLY:H | 12 | 0.44 |
| (1,1191) | 1:64:A:LEU:HD13 | 1:65:A:GLY:H | 12 | 0.44 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 20 | 0.44 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 13 | 0.44 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 16 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,765) | 1:106:A:ASP:H | 1:106:A:ASP:HB3 | 12 | 0.44 |
| (1,765) | 1:106:A:ASP:H | 1:106:A:ASP:HB3 | 14 | 0.44 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 4 | 0.44 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 4 | 0.44 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 4 | 0.44 |
| (1,587) | 1:46:A:VAL:HG21 | 1:47:A:ARG:H | 11 | 0.44 |
| (1,587) | 1:46:A:VAL:HG22 | 1:47:A:ARG:H | 11 | 0.44 |
| (1,587) | 1:46:A:VAL:HG23 | 1:47:A:ARG:H | 11 | 0.44 |
| (1,485) | 1:4:A:THR:H | 1:7:A:LYS:HB2 | 5 | 0.44 |
| (1,485) | 1:4:A:THR:H | 1:7:A:LYS:HB2 | 14 | 0.44 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 3 | 0.44 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 3 | 0.44 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 3 | 0.44 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 13 | 0.44 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 13 | 0.44 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 13 | 0.44 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 14 | 0.44 |
| (1,337) | 1:166:A:ASP:H | 1:176:A:GLN:HE21 | 19 | 0.44 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 14 | 0.44 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 17 | 0.44 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 17 | 0.44 |
| (1,132) | 1:56:A:MET:HB2 | 1:57:A:THR:H | 13 | 0.44 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 5 | 0.44 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 14 | 0.44 |
| (1,102) | 1:50:A:LEU:HD21 | 1:56:A:MET:H | 9 | 0.44 |
| (1,102) | 1:50:A:LEU:HD22 | 1:56:A:MET:H | 9 | 0.44 |
| (1,102) | 1:50:A:LEU:HD23 | 1:56:A:MET:H | 9 | 0.44 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 6 | 0.43 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 6 | 0.43 |
| (1,3443) | 1:73:A:GLN:HB2 | 1:125:A:TRP:HH2 | 13 | 0.43 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD11 | 3 | 0.43 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD12 | 3 | 0.43 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD13 | 3 | 0.43 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD11 | 3 | 0.43 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD12 | 3 | 0.43 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD13 | 3 | 0.43 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 19 | 0.43 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 19 | 0.43 |
| (1,3311) | 1:29:A:TYR:HD1 | 1:71:A:LEU:HB2 | 7 | 0.43 |
| (1,3311) | 1:29:A:TYR:HD2 | 1:71:A:LEU:HB2 | 7 | 0.43 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD11 | 7 | 0.43 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD12 | 7 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD13 | 7 | 0.43 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD11 | 7 | 0.43 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD12 | 7 | 0.43 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD13 | 7 | 0.43 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD11 | 7 | 0.43 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD12 | 7 | 0.43 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD13 | 7 | 0.43 |
| (1,3112) | 1:67:A:LEU:HA | 1:70:A:ASP:HB3 | 9 | 0.43 |
| (1,2935) | 1:75:A:TRP:HA | 1:78:A:ALA:HA | 19 | 0.43 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 17 | 0.43 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 17 | 0.43 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 17 | 0.43 |
| (1,2868) | 1:67:A:LEU:HD21 | 1:102:A:GLN:HA | 1 | 0.43 |
| (1,2868) | 1:67:A:LEU:HD22 | 1:102:A:GLN:HA | 1 | 0.43 |
| (1,2868) | 1:67:A:LEU:HD23 | 1:102:A:GLN:HA | 1 | 0.43 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 4 | 0.43 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 4 | 0.43 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 4 | 0.43 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 4 | 0.43 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 4 | 0.43 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 4 | 0.43 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 4 | 0.43 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 4 | 0.43 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 4 | 0.43 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG11 | 16 | 0.43 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG12 | 16 | 0.43 |
| (1,2772) | 1:78:A:ALA:H | 1:130:A:VAL:HG13 | 16 | 0.43 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD11 | 8 | 0.43 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD12 | 8 | 0.43 |
| (1,2687) | 1:184:A:LEU:HA | 1:184:A:LEU:HD13 | 8 | 0.43 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG21 | 4 | 0.43 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG22 | 4 | 0.43 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG23 | 4 | 0.43 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG21 | 4 | 0.43 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG22 | 4 | 0.43 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG23 | 4 | 0.43 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG21 | 4 | 0.43 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG22 | 4 | 0.43 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG23 | 4 | 0.43 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 2 | 0.43 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 2 | 0.43 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 2 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2587) | 1:95:A:VAL:HG11 | 1:101:A:VAL:HB | 4 | 0.43 |
| (1,2587) | 1:95:A:VAL:HG12 | 1:101:A:VAL:HB | 4 | 0.43 |
| (1,2587) | 1:95:A:VAL:HG13 | 1:101:A:VAL:HB | 4 | 0.43 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 4 | 0.43 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 4 | 0.43 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 4 | 0.43 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 12 | 0.43 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 12 | 0.43 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 12 | 0.43 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 12 | 0.43 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 12 | 0.43 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 12 | 0.43 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 12 | 0.43 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 12 | 0.43 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 12 | 0.43 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD21 | 7 | 0.43 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD22 | 7 | 0.43 |
| (1,2506) | 1:47:A:ARG:H | 1:50:A:LEU:HD23 | 7 | 0.43 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 4 | 0.43 |
| (1,2452) | 1:149:A:VAL:HG11 | 1:150:A:PRO:HG3 | 11 | 0.43 |
| (1,2452) | 1:149:A:VAL:HG12 | 1:150:A:PRO:HG3 | 11 | 0.43 |
| (1,2452) | 1:149:A:VAL:HG13 | 1:150:A:PRO:HG3 | 11 | 0.43 |
| (1,2452) | 1:149:A:VAL:HG21 | 1:150:A:PRO:HG3 | 11 | 0.43 |
| (1,2452) | 1:149:A:VAL:HG22 | 1:150:A:PRO:HG3 | 11 | 0.43 |
| (1,2452) | 1:149:A:VAL:HG23 | 1:150:A:PRO:HG3 | 11 | 0.43 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 20 | 0.43 |
| (1,2316) | 1:117:A:LYS:H | 1:117:A:LYS:HG2 | 4 | 0.43 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 18 | 0.43 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 18 | 0.43 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 18 | 0.43 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 19 | 0.43 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 19 | 0.43 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 19 | 0.43 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 20 | 0.43 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 20 | 0.43 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 20 | 0.43 |
| (1,2297) | 1:36:A:PHE:HA | 1:40:A:LEU:HD11 | 18 | 0.43 |
| (1,2297) | 1:36:A:PHE:HA | 1:40:A:LEU:HD12 | 18 | 0.43 |
| (1,2297) | 1:36:A:PHE:HA | 1:40:A:LEU:HD13 | 18 | 0.43 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 11 | 0.43 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 11 | 0.43 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 11 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 11 | 0.43 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 11 | 0.43 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 11 | 0.43 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB2 | 9 | 0.43 |
| (1,2187) | 1:42:A:VAL:HG21 | 1:43:A:SER:HB3 | 9 | 0.43 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB2 | 9 | 0.43 |
| (1,2187) | 1:42:A:VAL:HG22 | 1:43:A:SER:HB3 | 9 | 0.43 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB2 | 9 | 0.43 |
| (1,2187) | 1:42:A:VAL:HG23 | 1:43:A:SER:HB3 | 9 | 0.43 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 13 | 0.43 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 13 | 0.43 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 1 | 0.43 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 1 | 0.43 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 1 | 0.43 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 1 | 0.43 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 1 | 0.43 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 1 | 0.43 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 4 | 0.43 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 4 | 0.43 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 4 | 0.43 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 17 | 0.43 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 17 | 0.43 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 17 | 0.43 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 14 | 0.43 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB2 | 7 | 0.43 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB3 | 7 | 0.43 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 11 | 0.43 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 6 | 0.43 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 9 | 0.43 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 20 | 0.43 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 4 | 0.43 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 4 | 0.43 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 4 | 0.43 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 5 | 0.43 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 6 | 0.43 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 12 | 0.43 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 12 | 0.43 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 15 | 0.43 |
| (1,1813) | 1:160:A:LEU:HD21 | 1:180:A:THR:HB | 11 | 0.43 |
| (1,1813) | 1:160:A:LEU:HD22 | 1:180:A:THR:HB | 11 | 0.43 |
| (1,1813) | 1:160:A:LEU:HD23 | 1:180:A:THR:HB | 11 | 0.43 |
| (1,1778) | 1:72:A:THR:HB | 1:73:A:GLN:HB3 | 9 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1686) | 1:99:A:GLN:HG3 | 1:100:A:THR:H | 16 | 0.43 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB2 | 19 | 0.43 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB3 | 19 | 0.43 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 1 | 0.43 |
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 1 | 0.43 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 1 | 0.43 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 1 | 0.43 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 7 | 0.43 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 4 | 0.43 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 10 | 0.43 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 11 | 0.43 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 11 | 0.43 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 11 | 0.43 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG11 | 7 | 0.43 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG12 | 7 | 0.43 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG13 | 7 | 0.43 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 6 | 0.43 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 6 | 0.43 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 6 | 0.43 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 15 | 0.43 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 15 | 0.43 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 15 | 0.43 |
| (1,1427) | 1:143:A:ASP:HB2 | 1:145:A:GLN:HE22 | 7 | 0.43 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG21 | 14 | 0.43 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG22 | 14 | 0.43 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG23 | 14 | 0.43 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG21 | 14 | 0.43 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG22 | 14 | 0.43 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG23 | 14 | 0.43 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 1 | 0.43 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 1 | 0.43 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 1 | 0.43 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB2 | 14 | 0.43 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB3 | 14 | 0.43 |
| (1,1298) | 1:141:A:ALA:HA | 1:146:A:LEU:HB2 | 7 | 0.43 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 20 | 0.43 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 4 | 0.43 |
| (1,935) | 1:117:A:LYS:HB2 | 1:118:A:GLY:H | 1 | 0.43 |
| (1,778) | 1:51:A:PRO:HB3 | 1:54:A:THR:H | 12 | 0.43 |
| (1,765) | 1:106:A:ASP:H | 1:106:A:ASP:HB3 | 15 | 0.43 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 5 | 0.43 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 5 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 5 | 0.43 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 18 | 0.43 |
| (1,578) | 1:122:A:ASP:H | 1:122:A:ASP:HB3 | 2 | 0.43 |
| (1,578) | 1:122:A:ASP:H | 1:122:A:ASP:HB3 | 3 | 0.43 |
| (1,555) | 1:174:A:VAL:HG21 | 1:178:A:ALA:H | 1 | 0.43 |
| (1,555) | 1:174:A:VAL:HG22 | 1:178:A:ALA:H | 1 | 0.43 |
| (1,555) | 1:174:A:VAL:HG23 | 1:178:A:ALA:H | 1 | 0.43 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 5 | 0.43 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 10 | 0.43 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 18 | 0.43 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 18 | 0.43 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 18 | 0.43 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 18 | 0.43 |
| (1,438) | 1:60:A:HIS:HB2 | 1:75:A:TRP:H | 8 | 0.43 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 5 | 0.43 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 5 | 0.43 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 5 | 0.43 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 12 | 0.43 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 12 | 0.43 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 12 | 0.43 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 16 | 0.43 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 16 | 0.43 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 16 | 0.43 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 17 | 0.43 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 17 | 0.43 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 17 | 0.43 |
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 9 | 0.43 |
| (1,248) | 1:93:A:GLU:HG2 | 1:94:A:ALA:H | 17 | 0.43 |
| (1,248) | 1:93:A:GLU:HG3 | 1:94:A:ALA:H | 17 | 0.43 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 13 | 0.43 |
| (1,67) | 1:26:A:PHE:H | 1:59:A:TYR:H | 7 | 0.43 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE1 | 7 | 0.42 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE2 | 7 | 0.42 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE1 | 7 | 0.42 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE2 | 7 | 0.42 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE1 | 7 | 0.42 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE2 | 7 | 0.42 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB2 | 2 | 0.42 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB3 | 2 | 0.42 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB2 | 2 | 0.42 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB3 | 2 | 0.42 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 16 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3415) | 1:59:A:TYR:HD1 | 1:137:A:GLN:HG3 | 3 | 0.42 |
| (1,3415) | 1:59:A:TYR:HD2 | 1:137:A:GLN:HG3 | 3 | 0.42 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 17 | 0.42 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 17 | 0.42 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 17 | 0.42 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 17 | 0.42 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 17 | 0.42 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 17 | 0.42 |
| (1,3277) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA3 | 10 | 0.42 |
| (1,3277) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA3 | 10 | 0.42 |
| (1,3277) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA3 | 10 | 0.42 |
| (1,3250) | 1:68:A:GLY:HA3 | 1:71:A:LEU:HB2 | 7 | 0.42 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 5 | 0.42 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 5 | 0.42 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 5 | 0.42 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 5 | 0.42 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 5 | 0.42 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 5 | 0.42 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD21 | 8 | 0.42 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD22 | 8 | 0.42 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD23 | 8 | 0.42 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG11 | 15 | 0.42 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG12 | 15 | 0.42 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG13 | 15 | 0.42 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 11 | 0.42 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 11 | 0.42 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 11 | 0.42 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 19 | 0.42 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 19 | 0.42 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 19 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 5 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 5 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 5 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 5 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 5 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 5 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 5 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 5 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 5 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 20 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 20 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 20 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 20 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 20 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 20 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 20 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 20 | 0.42 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 20 | 0.42 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 1 | 0.42 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 1 | 0.42 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 1 | 0.42 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 1 | 0.42 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 1 | 0.42 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 1 | 0.42 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 5 | 0.42 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 5 | 0.42 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 5 | 0.42 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 15 | 0.42 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 18 | 0.42 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 15 | 0.42 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 15 | 0.42 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 15 | 0.42 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 15 | 0.42 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 15 | 0.42 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 15 | 0.42 |
| (1,2318) | 1:117:A:LYS:HG3 | 1:119:A:GLU:H | 12 | 0.42 |
| (1,2318) | 1:117:A:LYS:HG3 | 1:119:A:GLU:H | 15 | 0.42 |
| (1,2318) | 1:117:A:LYS:HG3 | 1:119:A:GLU:H | 20 | 0.42 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 14 | 0.42 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 14 | 0.42 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 14 | 0.42 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 18 | 0.42 |
| (1,2171) | 1:86:A:LYS:H | 1:87:A:ILE:HG12 | 5 | 0.42 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 15 | 0.42 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 4 | 0.42 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD1 | 7 | 0.42 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD2 | 7 | 0.42 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG11 | 4 | 0.42 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG12 | 4 | 0.42 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG13 | 4 | 0.42 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 8 | 0.42 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 17 | 0.42 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 15 | 0.42 |
| (1,1931) | 1:62:A:GLU:HB2 | 1:63:A:PHE:HB3 | 7 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1931) | 1:62:A:GLU:HB3 | 1:63:A:PHE:HB3 | 7 | 0.42 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB2 | 9 | 0.42 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB3 | 9 | 0.42 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB2 | 9 | 0.42 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB3 | 9 | 0.42 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB2 | 9 | 0.42 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB3 | 9 | 0.42 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB2 | 18 | 0.42 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB3 | 18 | 0.42 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB2 | 18 | 0.42 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB3 | 18 | 0.42 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB2 | 18 | 0.42 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB3 | 18 | 0.42 |
| (1,1867) | 1:37:A:GLU:HB2 | 1:38:A:GLU:HA | 14 | 0.42 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 7 | 0.42 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 8 | 0.42 |
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 8 | 0.42 |
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 8 | 0.42 |
| (1,1791) | 1:56:A:MET:HA | 1:56:A:MET:HG3 | 8 | 0.42 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG12 | 2 | 0.42 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG13 | 2 | 0.42 |
| (1,1686) | 1:99:A:GLN:HG3 | 1:100:A:THR:H | 6 | 0.42 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 10 | 0.42 |
| (1,1588) | 1:62:A:GLU:HA | 1:62:A:GLU:HG3 | 3 | 0.42 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 19 | 0.42 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 19 | 0.42 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 19 | 0.42 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 20 | 0.42 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 20 | 0.42 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 20 | 0.42 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 4 | 0.42 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 4 | 0.42 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 4 | 0.42 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 7 | 0.42 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 7 | 0.42 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 7 | 0.42 |
| (1,1474) | 1:161:A:ASN:HB2 | 1:161:A:ASN:HD22 | 18 | 0.42 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 13 | 0.42 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 13 | 0.42 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 13 | 0.42 |
| (1,1438) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HB2 | 1 | 0.42 |
| (1,1438) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HB2 | 1 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1438) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HB2 | 1 | 0.42 |
| (1,1438) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HB2 | 15 | 0.42 |
| (1,1438) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HB2 | 15 | 0.42 |
| (1,1438) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HB2 | 15 | 0.42 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 18 | 0.42 |
| (1,1339) | 1:10:A:ILE:HB | 1:159:A:GLN:HB2 | 14 | 0.42 |
| (1,1331) | 1:70:A:ASP:HB3 | 1:72:A:THR:H | 10 | 0.42 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 8 | 0.42 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 5 | 0.42 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 5 | 0.42 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 5 | 0.42 |
| (1,1116) | 1:61:A:VAL:HG11 | 1:63:A:PHE:H | 15 | 0.42 |
| (1,1116) | 1:61:A:VAL:HG12 | 1:63:A:PHE:H | 15 | 0.42 |
| (1,1116) | 1:61:A:VAL:HG13 | 1:63:A:PHE:H | 15 | 0.42 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 8 | 0.42 |
| (1,1005) | 1:46:A:VAL:HG21 | 1:48:A:GLN:H | 1 | 0.42 |
| (1,1005) | 1:46:A:VAL:HG22 | 1:48:A:GLN:H | 1 | 0.42 |
| (1,1005) | 1:46:A:VAL:HG23 | 1:48:A:GLN:H | 1 | 0.42 |
| (1,991) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HD22 | 17 | 0.42 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 7 | 0.42 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 9 | 0.42 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 9 | 0.42 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 9 | 0.42 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 17 | 0.42 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 17 | 0.42 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 17 | 0.42 |
| (1,799) | 1:49:A:LYS:HG2 | 1:179:A:ASP:H | 18 | 0.42 |
| (1,799) | 1:49:A:LYS:HG3 | 1:179:A:ASP:H | 18 | 0.42 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 3 | 0.42 |
| (1,765) | 1:106:A:ASP:H | 1:106:A:ASP:HB3 | 5 | 0.42 |
| (1,683) | 1:168:A:SER:H | 1:170:A:MET:HG2 | 4 | 0.42 |
| (1,632) | 1:87:A:ILE:HG21 | 1:91:A:MET:H | 3 | 0.42 |
| (1,632) | 1:87:A:ILE:HG22 | 1:91:A:MET:H | 3 | 0.42 |
| (1,632) | 1:87:A:ILE:HG23 | 1:91:A:MET:H | 3 | 0.42 |
| (1,632) | 1:87:A:ILE:HG21 | 1:91:A:MET:H | 18 | 0.42 |
| (1,632) | 1:87:A:ILE:HG22 | 1:91:A:MET:H | 18 | 0.42 |
| (1,632) | 1:87:A:ILE:HG23 | 1:91:A:MET:H | 18 | 0.42 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 20 | 0.42 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 7 | 0.42 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 7 | 0.42 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 7 | 0.42 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 14 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 14 | 0.42 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 14 | 0.42 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 17 | 0.42 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 17 | 0.42 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 17 | 0.42 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 19 | 0.42 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 19 | 0.42 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 19 | 0.42 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 11 | 0.42 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 11 | 0.42 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 11 | 0.42 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 13 | 0.42 |
| (1,259) | 1:69:A:LYS:HD2 | 1:70:A:ASP:H | 5 | 0.42 |
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 10 | 0.42 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 2 | 0.41 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 2 | 0.41 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 12 | 0.41 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 12 | 0.41 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 11 | 0.41 |
| (1,3252) | 1:29:A:TYR:HD1 | 1:68:A:GLY:HA3 | 9 | 0.41 |
| (1,3252) | 1:29:A:TYR:HD2 | 1:68:A:GLY:HA3 | 9 | 0.41 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD11 | 15 | 0.41 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD12 | 15 | 0.41 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD13 | 15 | 0.41 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD11 | 15 | 0.41 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD12 | 15 | 0.41 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD13 | 15 | 0.41 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD11 | 15 | 0.41 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD12 | 15 | 0.41 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD13 | 15 | 0.41 |
| (1,3112) | 1:67:A:LEU:HA | 1:70:A:ASP:HB3 | 5 | 0.41 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG21 | 4 | 0.41 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG22 | 4 | 0.41 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG23 | 4 | 0.41 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG21 | 4 | 0.41 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG22 | 4 | 0.41 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG23 | 4 | 0.41 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG21 | 4 | 0.41 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG22 | 4 | 0.41 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG23 | 4 | 0.41 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 2 | 0.41 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 2 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 2 | 0.41 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 2 | 0.41 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 2 | 0.41 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 2 | 0.41 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 2 | 0.41 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 2 | 0.41 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 2 | 0.41 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD21 | 6 | 0.41 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD22 | 6 | 0.41 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD23 | 6 | 0.41 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD21 | 6 | 0.41 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD22 | 6 | 0.41 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD23 | 6 | 0.41 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD21 | 6 | 0.41 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD22 | 6 | 0.41 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD23 | 6 | 0.41 |
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 12 | 0.41 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 15 | 0.41 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 7 | 0.41 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 7 | 0.41 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 7 | 0.41 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 13 | 0.41 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 13 | 0.41 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 13 | 0.41 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 17 | 0.41 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 17 | 0.41 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 17 | 0.41 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 17 | 0.41 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 17 | 0.41 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 17 | 0.41 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG21 | 10 | 0.41 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG22 | 10 | 0.41 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG23 | 10 | 0.41 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG21 | 10 | 0.41 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG22 | 10 | 0.41 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG23 | 10 | 0.41 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG21 | 10 | 0.41 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG22 | 10 | 0.41 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG23 | 10 | 0.41 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 3 | 0.41 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 3 | 0.41 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 3 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 3 | 0.41 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 3 | 0.41 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 3 | 0.41 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 3 | 0.41 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 3 | 0.41 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 3 | 0.41 |
| (1,2456) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HA | 13 | 0.41 |
| (1,2456) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HA | 13 | 0.41 |
| (1,2456) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HA | 13 | 0.41 |
| (1,2452) | 1:149:A:VAL:HG11 | 1:150:A:PRO:HG3 | 16 | 0.41 |
| (1,2452) | 1:149:A:VAL:HG12 | 1:150:A:PRO:HG3 | 16 | 0.41 |
| (1,2452) | 1:149:A:VAL:HG13 | 1:150:A:PRO:HG3 | 16 | 0.41 |
| (1,2452) | 1:149:A:VAL:HG21 | 1:150:A:PRO:HG3 | 16 | 0.41 |
| (1,2452) | 1:149:A:VAL:HG22 | 1:150:A:PRO:HG3 | 16 | 0.41 |
| (1,2452) | 1:149:A:VAL:HG23 | 1:150:A:PRO:HG3 | 16 | 0.41 |
| (1,2318) | 1:117:A:LYS:HG3 | 1:119:A:GLU:H | 2 | 0.41 |
| (1,2318) | 1:117:A:LYS:HG3 | 1:119:A:GLU:H | 4 | 0.41 |
| (1,2318) | 1:117:A:LYS:HG3 | 1:119:A:GLU:H | 8 | 0.41 |
| (1,2318) | 1:117:A:LYS:HG3 | 1:119:A:GLU:H | 17 | 0.41 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 4 | 0.41 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 4 | 0.41 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 4 | 0.41 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 11 | 0.41 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 11 | 0.41 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 11 | 0.41 |
| (1,2291) | 1:117:A:LYS:HG3 | 1:120:A:ASP:H | 15 | 0.41 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 20 | 0.41 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 20 | 0.41 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 20 | 0.41 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 10 | 0.41 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 9 | 0.41 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 9 | 0.41 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD1 | 19 | 0.41 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD2 | 19 | 0.41 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 9 | 0.41 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 6 | 0.41 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 11 | 0.41 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 20 | 0.41 |
| (1,1980) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HD3 | 11 | 0.41 |
| (1,1980) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HD3 | 11 | 0.41 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 13 | 0.41 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 18 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 10 | 0.41 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 10 | 0.41 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 10 | 0.41 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 10 | 0.41 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 10 | 0.41 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 10 | 0.41 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 2 | 0.41 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 3 | 0.41 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 14 | 0.41 |
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 15 | 0.41 |
| (1,1722) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HG2 | 7 | 0.41 |
| (1,1722) | 1:145:A:GLN:HE22 | 1:147:A:GLN:HG3 | 7 | 0.41 |
| (1,1686) | 1:99:A:GLN:HG3 | 1:100:A:THR:H | 14 | 0.41 |
| (1,1603) | 1:62:A:GLU:HG2 | 1:63:A:PHE:H | 7 | 0.41 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 3 | 0.41 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 6 | 0.41 |
| (1,1581) | 1:62:A:GLU:HA | 1:62:A:GLU:HG2 | 16 | 0.41 |
| (1,1549) | 1:186:A:GLU:HG2 | 1:187:A:LYS:HD3 | 8 | 0.41 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 4 | 0.41 |
| (1,1430) | 1:117:A:LYS:H | 1:120:A:ASP:HB2 | 12 | 0.41 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 2 | 0.41 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 2 | 0.41 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 2 | 0.41 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 5 | 0.41 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 7 | 0.41 |
| (1,1331) | 1:70:A:ASP:HB3 | 1:72:A:THR:H | 4 | 0.41 |
| (1,1294) | 1:71:A:LEU:HB2 | 1:74:A:ALA:H | 1 | 0.41 |
| (1,1265) | 1:64:A:LEU:HB3 | 1:65:A:GLY:HA2 | 19 | 0.41 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 15 | 0.41 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 18 | 0.41 |
| (1,1164) | 1:27:A:SER:H | 1:30:A:CYS:HB3 | 2 | 0.41 |
| (1,1164) | 1:27:A:SER:H | 1:30:A:CYS:HB3 | 18 | 0.41 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG21 | 1 | 0.41 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG22 | 1 | 0.41 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG23 | 1 | 0.41 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 11 | 0.41 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 1 | 0.41 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 1 | 0.41 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 1 | 0.41 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 18 | 0.41 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 18 | 0.41 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 18 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD21 | 5 | 0.41 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD22 | 5 | 0.41 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD23 | 5 | 0.41 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 1 | 0.41 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 1 | 0.41 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 1 | 0.41 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 10 | 0.41 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 10 | 0.41 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 10 | 0.41 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 8 | 0.41 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 8 | 0.41 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 8 | 0.41 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 2 | 0.41 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 10 | 0.41 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 9 | 0.41 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 9 | 0.41 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 9 | 0.41 |
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 16 | 0.41 |
| (1,578) | 1:122:A:ASP:H | 1:122:A:ASP:HB3 | 6 | 0.41 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 4 | 0.41 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 4 | 0.41 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 4 | 0.41 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 18 | 0.41 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 18 | 0.41 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 18 | 0.41 |
| (1,498) | 1:77:A:VAL:HG11 | 1:124:A:ALA:H | 4 | 0.41 |
| (1,498) | 1:77:A:VAL:HG12 | 1:124:A:ALA:H | 4 | 0.41 |
| (1,498) | 1:77:A:VAL:HG13 | 1:124:A:ALA:H | 4 | 0.41 |
| (1,438) | 1:60:A:HIS:HB2 | 1:75:A:TRP:H | 11 | 0.41 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 8 | 0.41 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 8 | 0.41 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 8 | 0.41 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 11 | 0.41 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 11 | 0.41 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 11 | 0.41 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 18 | 0.41 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 18 | 0.41 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 18 | 0.41 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 9 | 0.41 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 11 | 0.41 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 11 | 0.41 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 11 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,241) | 1:70:A:ASP:HB2 | 1:74:A:ALA:H | 15 | 0.41 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG11 | 5 | 0.41 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG12 | 5 | 0.41 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG13 | 5 | 0.41 |
| (1,78) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 3 | 0.41 |
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 9 | 0.41 |
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 18 | 0.41 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE1 | 18 | 0.4 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE2 | 18 | 0.4 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE1 | 18 | 0.4 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE2 | 18 | 0.4 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE1 | 18 | 0.4 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE2 | 18 | 0.4 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 20 | 0.4 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 20 | 0.4 |
| (1,3480) | 1:32:A:HIS:HD2 | 1:150:A:PRO:HG3 | 7 | 0.4 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG2 | 9 | 0.4 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG3 | 9 | 0.4 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE1 | 18 | 0.4 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE2 | 18 | 0.4 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 2 | 0.4 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 2 | 0.4 |
| (1,3269) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA2 | 11 | 0.4 |
| (1,3269) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA2 | 11 | 0.4 |
| (1,3269) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA2 | 11 | 0.4 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 12 | 0.4 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 12 | 0.4 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 12 | 0.4 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 12 | 0.4 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 12 | 0.4 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 12 | 0.4 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG21 | 9 | 0.4 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG22 | 9 | 0.4 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG23 | 9 | 0.4 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG21 | 9 | 0.4 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG22 | 9 | 0.4 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG23 | 9 | 0.4 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG21 | 9 | 0.4 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG22 | 9 | 0.4 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG23 | 9 | 0.4 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 16 | 0.4 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 16 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 16 | 0.4 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD21 | 18 | 0.4 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD22 | 18 | 0.4 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD23 | 18 | 0.4 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG11 | 9 | 0.4 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG12 | 9 | 0.4 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG13 | 9 | 0.4 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG11 | 12 | 0.4 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG12 | 12 | 0.4 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG13 | 12 | 0.4 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 1 | 0.4 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 1 | 0.4 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 1 | 0.4 |
| (1,2838) | 1:34:A:TYR:HE1 | 1:38:A:GLU:HA | 4 | 0.4 |
| (1,2838) | 1:34:A:TYR:HE2 | 1:38:A:GLU:HA | 4 | 0.4 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 14 | 0.4 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 14 | 0.4 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 14 | 0.4 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 4 | 0.4 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 4 | 0.4 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 4 | 0.4 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 1 | 0.4 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 1 | 0.4 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 1 | 0.4 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 17 | 0.4 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 17 | 0.4 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 17 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 18 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 18 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 18 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 18 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 18 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 18 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 18 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 18 | 0.4 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 18 | 0.4 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 5 | 0.4 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 16 | 0.4 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 16 | 0.4 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 16 | 0.4 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 2 | 0.4 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 2 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 2 | 0.4 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 2 | 0.4 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 2 | 0.4 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 2 | 0.4 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 7 | 0.4 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 14 | 0.4 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 19 | 0.4 |
| (1,2318) | 1:117:A:LYS:HG3 | 1:119:A:GLU:H | 3 | 0.4 |
| (1,2318) | 1:117:A:LYS:HG3 | 1:119:A:GLU:H | 10 | 0.4 |
| (1,2318) | 1:117:A:LYS:HG3 | 1:119:A:GLU:H | 11 | 0.4 |
| (1,2318) | 1:117:A:LYS:HG3 | 1:119:A:GLU:H | 18 | 0.4 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 4 | 0.4 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 4 | 0.4 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 4 | 0.4 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 7 | 0.4 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 2 | 0.4 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 8 | 0.4 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 11 | 0.4 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 11 | 0.4 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 11 | 0.4 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 4 | 0.4 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 10 | 0.4 |
| (1,2159) | 1:76:A:ALA:HA | 1:79:A:ILE:HG12 | 10 | 0.4 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 1 | 0.4 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 1 | 0.4 |
| (1,2017) | 1:117:A:LYS:HD3 | 1:120:A:ASP:H | 16 | 0.4 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 14 | 0.4 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 19 | 0.4 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 19 | 0.4 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 19 | 0.4 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB2 | 8 | 0.4 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB3 | 8 | 0.4 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB2 | 8 | 0.4 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB3 | 8 | 0.4 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB2 | 8 | 0.4 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB3 | 8 | 0.4 |
| (1,1860) | 1:101:A:VAL:HB | 1:106:A:ASP:HB3 | 7 | 0.4 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 9 | 0.4 |
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 8 | 0.4 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD1 | 4 | 0.4 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD2 | 4 | 0.4 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG2 | 6 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG3 | 6 | 0.4 |
| (1,1686) | 1:99:A:GLN:HG3 | 1:100:A:THR:H | 5 | 0.4 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 8 | 0.4 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 8 | 0.4 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 8 | 0.4 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 4 | 0.4 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 18 | 0.4 |
| (1,1578) | 1:118:A:GLY:H | 1:119:A:GLU:HG3 | 8 | 0.4 |
| (1,1565) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 2 | 0.4 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 9 | 0.4 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 9 | 0.4 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 16 | 0.4 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 15 | 0.4 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 3 | 0.4 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 16 | 0.4 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 3 | 0.4 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 9 | 0.4 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 5 | 0.4 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 5 | 0.4 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 5 | 0.4 |
| (1,1444) | 1:83:A:VAL:HA | 1:85:A:ASP:HB2 | 9 | 0.4 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 17 | 0.4 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 17 | 0.4 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 17 | 0.4 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 3 | 0.4 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 3 | 0.4 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 3 | 0.4 |
| (1,1438) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HB2 | 13 | 0.4 |
| (1,1438) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HB2 | 13 | 0.4 |
| (1,1438) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HB2 | 13 | 0.4 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 3 | 0.4 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 3 | 0.4 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 3 | 0.4 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 3 | 0.4 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 11 | 0.4 |
| (1,1185) | 1:29:A:TYR:HE1 | 1:68:A:GLY:H | 10 | 0.4 |
| (1,1185) | 1:29:A:TYR:HE2 | 1:68:A:GLY:H | 10 | 0.4 |
| (1,1148) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE22 | 16 | 0.4 |
| (1,1148) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE22 | 16 | 0.4 |
| (1,1148) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE22 | 16 | 0.4 |
| (1,1134) | 1:73:A:GLN:HE21 | 1:126:A:ASN:H | 18 | 0.4 |
| (1,1080) | 1:34:A:TYR:HD1 | 1:38:A:GLU:H | 1 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,991) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HD22 | 11 | 0.4 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 5 | 0.4 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 11 | 0.4 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 11 | 0.4 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 11 | 0.4 |
| (1,883) | 1:49:A:LYS:H | 1:49:A:LYS:HD3 | 2 | 0.4 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 15 | 0.4 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 15 | 0.4 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 15 | 0.4 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 7 | 0.4 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 10 | 0.4 |
| (1,606) | 1:137:A:GLN:H | 1:137:A:GLN:HG2 | 20 | 0.4 |
| (1,578) | 1:122:A:ASP:H | 1:122:A:ASP:HB3 | 14 | 0.4 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 12 | 0.4 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 12 | 0.4 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 12 | 0.4 |
| (1,438) | 1:60:A:HIS:HB2 | 1:75:A:TRP:H | 4 | 0.4 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 2 | 0.4 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 2 | 0.4 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 2 | 0.4 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 10 | 0.4 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 10 | 0.4 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 10 | 0.4 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 15 | 0.4 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 15 | 0.4 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 15 | 0.4 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 20 | 0.4 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 20 | 0.4 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 20 | 0.4 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 13 | 0.4 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 13 | 0.4 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 13 | 0.4 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 15 | 0.4 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 15 | 0.4 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 15 | 0.4 |
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 8 | 0.4 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 8 | 0.4 |
| (1,241) | 1:70:A:ASP:HB2 | 1:74:A:ALA:H | 5 | 0.4 |
| (1,127) | 1:105:A:ALA:H | 1:107:A:ILE:HB | 1 | 0.4 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 17 | 0.39 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 17 | 0.39 |
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 19 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 19 | 0.39 |
| (1,3311) | 1:29:A:TYR:HD1 | 1:71:A:LEU:HB2 | 8 | 0.39 |
| (1,3311) | 1:29:A:TYR:HD2 | 1:71:A:LEU:HB2 | 8 | 0.39 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 18 | 0.39 |
| (1,3277) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA3 | 16 | 0.39 |
| (1,3277) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA3 | 16 | 0.39 |
| (1,3277) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA3 | 16 | 0.39 |
| (1,3274) | 1:118:A:GLY:HA3 | 1:121:A:TYR:H | 5 | 0.39 |
| (1,3269) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA2 | 2 | 0.39 |
| (1,3269) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA2 | 2 | 0.39 |
| (1,3269) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA2 | 2 | 0.39 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 9 | 0.39 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 9 | 0.39 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 9 | 0.39 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 9 | 0.39 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 9 | 0.39 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 9 | 0.39 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 20 | 0.39 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 20 | 0.39 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 20 | 0.39 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 2 | 0.39 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 5 | 0.39 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 5 | 0.39 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 5 | 0.39 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG11 | 7 | 0.39 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG12 | 7 | 0.39 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG13 | 7 | 0.39 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 3 | 0.39 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 3 | 0.39 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 3 | 0.39 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 3 | 0.39 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 3 | 0.39 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 3 | 0.39 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 15 | 0.39 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 15 | 0.39 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 15 | 0.39 |
| (1,2632) | 1:101:A:VAL:HG21 | 1:107:A:ILE:H | 8 | 0.39 |
| (1,2632) | 1:101:A:VAL:HG22 | 1:107:A:ILE:H | 8 | 0.39 |
| (1,2632) | 1:101:A:VAL:HG23 | 1:107:A:ILE:H | 8 | 0.39 |
| (1,2621) | 1:101:A:VAL:HG21 | 1:106:A:ASP:H | 8 | 0.39 |
| (1,2621) | 1:101:A:VAL:HG22 | 1:106:A:ASP:H | 8 | 0.39 |
| (1,2621) | 1:101:A:VAL:HG23 | 1:106:A:ASP:H | 8 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG21 | 3 | 0.39 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG22 | 3 | 0.39 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG23 | 3 | 0.39 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG21 | 3 | 0.39 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG22 | 3 | 0.39 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG23 | 3 | 0.39 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG21 | 3 | 0.39 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG22 | 3 | 0.39 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG23 | 3 | 0.39 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 4 | 0.39 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 12 | 0.39 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 12 | 0.39 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 12 | 0.39 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 12 | 0.39 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 12 | 0.39 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 12 | 0.39 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 17 | 0.39 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 15 | 0.39 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 8 | 0.39 |
| (1,2318) | 1:117:A:LYS:HG3 | 1:119:A:GLU:H | 9 | 0.39 |
| (1,2316) | 1:117:A:LYS:H | 1:117:A:LYS:HG2 | 15 | 0.39 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 12 | 0.39 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 12 | 0.39 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 12 | 0.39 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 7 | 0.39 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 7 | 0.39 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 7 | 0.39 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 4 | 0.39 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 6 | 0.39 |
| (1,2195) | 1:66:A:PRO:HD2 | 1:67:A:LEU:HG | 18 | 0.39 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 14 | 0.39 |
| (1,2168) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HG2 | 18 | 0.39 |
| (1,2168) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HG2 | 18 | 0.39 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 2 | 0.39 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 2 | 0.39 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG21 | 4 | 0.39 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG22 | 4 | 0.39 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG23 | 4 | 0.39 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG21 | 4 | 0.39 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG22 | 4 | 0.39 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG23 | 4 | 0.39 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG21 | 4 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG22 | 4 | 0.39 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG23 | 4 | 0.39 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 8 | 0.39 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 2 | 0.39 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 16 | 0.39 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 19 | 0.39 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 3 | 0.39 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 14 | 0.39 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 1 | 0.39 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 1 | 0.39 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 1 | 0.39 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 1 | 0.39 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 1 | 0.39 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 1 | 0.39 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 13 | 0.39 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 13 | 0.39 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 13 | 0.39 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 13 | 0.39 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 13 | 0.39 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 13 | 0.39 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 5 | 0.39 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 5 | 0.39 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 5 | 0.39 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 6 | 0.39 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 6 | 0.39 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 6 | 0.39 |
| (1,1843) | 1:60:A:HIS:HB2 | 1:72:A:THR:HA | 12 | 0.39 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 19 | 0.39 |
| (1,1813) | 1:160:A:LEU:HD21 | 1:180:A:THR:HB | 2 | 0.39 |
| (1,1813) | 1:160:A:LEU:HD22 | 1:180:A:THR:HB | 2 | 0.39 |
| (1,1813) | 1:160:A:LEU:HD23 | 1:180:A:THR:HB | 2 | 0.39 |
| (1,1694) | 1:136:A:GLN:HG2 | 1:137:A:GLN:H | 12 | 0.39 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG2 | 18 | 0.39 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG3 | 18 | 0.39 |
| (1,1663) | 1:72:A:THR:HG21 | 1:138:A:GLU:HG3 | 15 | 0.39 |
| (1,1663) | 1:72:A:THR:HG22 | 1:138:A:GLU:HG3 | 15 | 0.39 |
| (1,1663) | 1:72:A:THR:HG23 | 1:138:A:GLU:HG3 | 15 | 0.39 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 11 | 0.39 |
| (1,1606) | 1:52:A:GLU:HG2 | 1:53:A:GLY:HA3 | 11 | 0.39 |
| (1,1606) | 1:52:A:GLU:HG3 | 1:53:A:GLY:HA3 | 11 | 0.39 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 8 | 0.39 |
| (1,1565) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 14 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 2 | 0.39 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 2 | 0.39 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 2 | 0.39 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 10 | 0.39 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 13 | 0.39 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 4 | 0.39 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 4 | 0.39 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 4 | 0.39 |
| (1,1402) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HA | 16 | 0.39 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 6 | 0.39 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 6 | 0.39 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 6 | 0.39 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE2 | 2 | 0.39 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE3 | 2 | 0.39 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE2 | 2 | 0.39 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE3 | 2 | 0.39 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE2 | 2 | 0.39 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE3 | 2 | 0.39 |
| (1,1265) | 1:64:A:LEU:HB3 | 1:65:A:GLY:HA2 | 1 | 0.39 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 10 | 0.39 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 14 | 0.39 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 17 | 0.39 |
| (1,1191) | 1:64:A:LEU:HD11 | 1:65:A:GLY:H | 11 | 0.39 |
| (1,1191) | 1:64:A:LEU:HD12 | 1:65:A:GLY:H | 11 | 0.39 |
| (1,1191) | 1:64:A:LEU:HD13 | 1:65:A:GLY:H | 11 | 0.39 |
| (1,991) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HD22 | 7 | 0.39 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 1 | 0.39 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 16 | 0.39 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 17 | 0.39 |
| (1,883) | 1:49:A:LYS:H | 1:49:A:LYS:HD3 | 9 | 0.39 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 7 | 0.39 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 7 | 0.39 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 7 | 0.39 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 11 | 0.39 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 11 | 0.39 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 11 | 0.39 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 12 | 0.39 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 12 | 0.39 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 12 | 0.39 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 14 | 0.39 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 14 | 0.39 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 14 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 10 | 0.39 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 4 | 0.39 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 19 | 0.39 |
| (1,606) | 1:137:A:GLN:H | 1:137:A:GLN:HG2 | 11 | 0.39 |
| (1,599) | 1:183:A:GLN:HB3 | 1:184:A:LEU:H | 8 | 0.39 |
| (1,578) | 1:122:A:ASP:H | 1:122:A:ASP:HB3 | 8 | 0.39 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 19 | 0.39 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 19 | 0.39 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 19 | 0.39 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 15 | 0.39 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 15 | 0.39 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 15 | 0.39 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 6 | 0.39 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 6 | 0.39 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 6 | 0.39 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 9 | 0.39 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 9 | 0.39 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 9 | 0.39 |
| (1,401) | 1:117:A:LYS:HB2 | 1:120:A:ASP:H | 12 | 0.39 |
| (1,367) | 1:110:A:VAL:HG21 | 1:114:A:ALA:H | 5 | 0.39 |
| (1,367) | 1:110:A:VAL:HG22 | 1:114:A:ALA:H | 5 | 0.39 |
| (1,367) | 1:110:A:VAL:HG23 | 1:114:A:ALA:H | 5 | 0.39 |
| (1,285) | 1:152:A:MET:H | 1:152:A:MET:HB3 | 2 | 0.39 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 6 | 0.39 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 6 | 0.39 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 6 | 0.39 |
| (1,185) | 1:59:A:TYR:HB2 | 1:60:A:HIS:H | 3 | 0.39 |
| (1,165) | 1:67:A:LEU:H | 1:69:A:LYS:H | 4 | 0.39 |
| (1,132) | 1:56:A:MET:HB2 | 1:57:A:THR:H | 7 | 0.39 |
| (1,127) | 1:105:A:ALA:H | 1:107:A:ILE:HB | 7 | 0.39 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG11 | 13 | 0.39 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG12 | 13 | 0.39 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG13 | 13 | 0.39 |
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 3 | 0.39 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 18 | 0.38 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 18 | 0.38 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 18 | 0.38 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 18 | 0.38 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 18 | 0.38 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 18 | 0.38 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 6 | 0.38 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 16 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 4 | 0.38 |
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 4 | 0.38 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE1 | 1 | 0.38 |
| (1,3405) | 1:37:A:GLU:HB2 | 1:92:A:PHE:HE2 | 1 | 0.38 |
| (1,3297) | 1:23:A:LEU:HB2 | 1:153:A:TYR:H | 10 | 0.38 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB1 | 13 | 0.38 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB2 | 13 | 0.38 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB3 | 13 | 0.38 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB1 | 14 | 0.38 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB2 | 14 | 0.38 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB3 | 14 | 0.38 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD21 | 16 | 0.38 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD22 | 16 | 0.38 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD23 | 16 | 0.38 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 12 | 0.38 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 12 | 0.38 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 12 | 0.38 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 12 | 0.38 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 12 | 0.38 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 12 | 0.38 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 12 | 0.38 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 12 | 0.38 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 12 | 0.38 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 3 | 0.38 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 3 | 0.38 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 3 | 0.38 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 5 | 0.38 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 5 | 0.38 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 5 | 0.38 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 16 | 0.38 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 16 | 0.38 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 16 | 0.38 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 9 | 0.38 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 9 | 0.38 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 9 | 0.38 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 9 | 0.38 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 9 | 0.38 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 9 | 0.38 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 10 | 0.38 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 10 | 0.38 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 10 | 0.38 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 10 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 10 | 0.38 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 10 | 0.38 |
| (1,2621) | 1:101:A:VAL:HG21 | 1:106:A:ASP:H | 5 | 0.38 |
| (1,2621) | 1:101:A:VAL:HG22 | 1:106:A:ASP:H | 5 | 0.38 |
| (1,2621) | 1:101:A:VAL:HG23 | 1:106:A:ASP:H | 5 | 0.38 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 9 | 0.38 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 9 | 0.38 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 9 | 0.38 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 11 | 0.38 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 11 | 0.38 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 11 | 0.38 |
| (1,2588) | 1:70:A:ASP:HA | 1:72:A:THR:H | 1 | 0.38 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG11 | 18 | 0.38 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG12 | 18 | 0.38 |
| (1,2560) | 1:40:A:LEU:HD21 | 1:174:A:VAL:HG13 | 18 | 0.38 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG11 | 18 | 0.38 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG12 | 18 | 0.38 |
| (1,2560) | 1:40:A:LEU:HD22 | 1:174:A:VAL:HG13 | 18 | 0.38 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG11 | 18 | 0.38 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG12 | 18 | 0.38 |
| (1,2560) | 1:40:A:LEU:HD23 | 1:174:A:VAL:HG13 | 18 | 0.38 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 2 | 0.38 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 2 | 0.38 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 2 | 0.38 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 2 | 0.38 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 2 | 0.38 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 2 | 0.38 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 2 | 0.38 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 2 | 0.38 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 2 | 0.38 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 16 | 0.38 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 4 | 0.38 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 4 | 0.38 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 4 | 0.38 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 5 | 0.38 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 5 | 0.38 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 5 | 0.38 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 20 | 0.38 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 13 | 0.38 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 5 | 0.38 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 18 | 0.38 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 1 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 16 | 0.38 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 12 | 0.38 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 12 | 0.38 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 12 | 0.38 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 12 | 0.38 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 12 | 0.38 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 12 | 0.38 |
| (1,2118) | 1:10:A:ILE:HG13 | 1:159:A:GLN:H | 5 | 0.38 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 3 | 0.38 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 16 | 0.38 |
| (1,1935) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HA | 3 | 0.38 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 9 | 0.38 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 9 | 0.38 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 9 | 0.38 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 10 | 0.38 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 10 | 0.38 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 10 | 0.38 |
| (1,1813) | 1:160:A:LEU:HD21 | 1:180:A:THR:HB | 6 | 0.38 |
| (1,1813) | 1:160:A:LEU:HD22 | 1:180:A:THR:HB | 6 | 0.38 |
| (1,1813) | 1:160:A:LEU:HD23 | 1:180:A:THR:HB | 6 | 0.38 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 7 | 0.38 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 7 | 0.38 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 7 | 0.38 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 7 | 0.38 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 7 | 0.38 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 7 | 0.38 |
| (1,1699) | 1:135:A:ALA:HB1 | 1:136:A:GLN:HG2 | 4 | 0.38 |
| (1,1699) | 1:135:A:ALA:HB2 | 1:136:A:GLN:HG2 | 4 | 0.38 |
| (1,1699) | 1:135:A:ALA:HB3 | 1:136:A:GLN:HG2 | 4 | 0.38 |
| (1,1694) | 1:136:A:GLN:HG2 | 1:137:A:GLN:H | 15 | 0.38 |
| (1,1694) | 1:136:A:GLN:HG2 | 1:137:A:GLN:H | 20 | 0.38 |
| (1,1606) | 1:52:A:GLU:HG2 | 1:53:A:GLY:HA3 | 19 | 0.38 |
| (1,1606) | 1:52:A:GLU:HG3 | 1:53:A:GLY:HA3 | 19 | 0.38 |
| (1,1588) | 1:62:A:GLU:HA | 1:62:A:GLU:HG3 | 2 | 0.38 |
| (1,1545) | 1:186:A:GLU:HG3 | 1:187:A:LYS:HD3 | 8 | 0.38 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 1 | 0.38 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG11 | 11 | 0.38 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG12 | 11 | 0.38 |
| (1,1495) | 1:128:A:PHE:HB2 | 1:129:A:VAL:HG13 | 11 | 0.38 |
| (1,1485) | 1:28:A:PHE:HB2 | 1:95:A:VAL:HB | 8 | 0.38 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 8 | 0.38 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 14 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 8 | 0.38 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 8 | 0.38 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 8 | 0.38 |
| (1,1409) | 1:67:A:LEU:HB2 | 1:70:A:ASP:HB3 | 4 | 0.38 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 11 | 0.38 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 11 | 0.38 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 11 | 0.38 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 12 | 0.38 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 12 | 0.38 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 12 | 0.38 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 2 | 0.38 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 8 | 0.38 |
| (1,1294) | 1:71:A:LEU:HB2 | 1:74:A:ALA:H | 13 | 0.38 |
| (1,1258) | 1:163:A:GLN:HG2 | 1:164:A:GLY:HA3 | 11 | 0.38 |
| (1,1258) | 1:163:A:GLN:HG3 | 1:164:A:GLY:HA3 | 11 | 0.38 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 1 | 0.38 |
| (1,1005) | 1:46:A:VAL:HG21 | 1:48:A:GLN:H | 12 | 0.38 |
| (1,1005) | 1:46:A:VAL:HG22 | 1:48:A:GLN:H | 12 | 0.38 |
| (1,1005) | 1:46:A:VAL:HG23 | 1:48:A:GLN:H | 12 | 0.38 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG21 | 4 | 0.38 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG22 | 4 | 0.38 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG23 | 4 | 0.38 |
| (1,979) | 1:29:A:TYR:H | 1:71:A:LEU:HD11 | 7 | 0.38 |
| (1,979) | 1:29:A:TYR:H | 1:71:A:LEU:HD12 | 7 | 0.38 |
| (1,979) | 1:29:A:TYR:H | 1:71:A:LEU:HD13 | 7 | 0.38 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 14 | 0.38 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 18 | 0.38 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 18 | 0.38 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 20 | 0.38 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 20 | 0.38 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 20 | 0.38 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 5 | 0.38 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 5 | 0.38 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 5 | 0.38 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 6 | 0.38 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 6 | 0.38 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 6 | 0.38 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 19 | 0.38 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 19 | 0.38 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 19 | 0.38 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 17 | 0.38 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 7 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,683) | 1:168:A:SER:H | 1:170:A:MET:HG2 | 18 | 0.38 |
| (1,578) | 1:122:A:ASP:H | 1:122:A:ASP:HB3 | 13 | 0.38 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 15 | 0.38 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 15 | 0.38 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 15 | 0.38 |
| (1,498) | 1:77:A:VAL:HG11 | 1:124:A:ALA:H | 12 | 0.38 |
| (1,498) | 1:77:A:VAL:HG12 | 1:124:A:ALA:H | 12 | 0.38 |
| (1,498) | 1:77:A:VAL:HG13 | 1:124:A:ALA:H | 12 | 0.38 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 12 | 0.38 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 12 | 0.38 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 12 | 0.38 |
| (1,438) | 1:60:A:HIS:HB2 | 1:75:A:TRP:H | 20 | 0.38 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 1 | 0.38 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 1 | 0.38 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 1 | 0.38 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG11 | 4 | 0.38 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG12 | 4 | 0.38 |
| (1,428) | 1:185:A:VAL:H | 1:185:A:VAL:HG13 | 4 | 0.38 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 8 | 0.38 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 7 | 0.38 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 7 | 0.38 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 7 | 0.38 |
| (1,337) | 1:166:A:ASP:H | 1:176:A:GLN:HE21 | 15 | 0.38 |
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 18 | 0.38 |
| (1,259) | 1:69:A:LYS:HD2 | 1:70:A:ASP:H | 9 | 0.38 |
| (1,163) | 1:69:A:LYS:H | 1:70:A:ASP:HB3 | 7 | 0.38 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 11 | 0.38 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 11 | 0.38 |
| (1,134) | 1:23:A:LEU:HD21 | 1:57:A:THR:H | 19 | 0.38 |
| (1,134) | 1:23:A:LEU:HD22 | 1:57:A:THR:H | 19 | 0.38 |
| (1,134) | 1:23:A:LEU:HD23 | 1:57:A:THR:H | 19 | 0.38 |
| (1,87) | 1:6:A:GLY:HA3 | 1:11:A:THR:H | 9 | 0.38 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 16 | 0.38 |
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 14 | 0.38 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 11 | 0.37 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 11 | 0.37 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 11 | 0.37 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 11 | 0.37 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 11 | 0.37 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 11 | 0.37 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB2 | 20 | 0.37 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB3 | 20 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB2 | 20 | 0.37 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB3 | 20 | 0.37 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 9 | 0.37 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 9 | 0.37 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 13 | 0.37 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 13 | 0.37 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 2 | 0.37 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 2 | 0.37 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG2 | 7 | 0.37 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG3 | 7 | 0.37 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 11 | 0.37 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 11 | 0.37 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 10 | 0.37 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 10 | 0.37 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 10 | 0.37 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 10 | 0.37 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 10 | 0.37 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 10 | 0.37 |
| (1,3278) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA3 | 11 | 0.37 |
| (1,3269) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA2 | 3 | 0.37 |
| (1,3269) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA2 | 3 | 0.37 |
| (1,3269) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA2 | 3 | 0.37 |
| (1,3250) | 1:68:A:GLY:HA3 | 1:71:A:LEU:HB2 | 16 | 0.37 |
| (1,3112) | 1:67:A:LEU:HA | 1:70:A:ASP:HB3 | 4 | 0.37 |
| (1,3112) | 1:67:A:LEU:HA | 1:70:A:ASP:HB3 | 10 | 0.37 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB1 | 1 | 0.37 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB2 | 1 | 0.37 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB3 | 1 | 0.37 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB1 | 1 | 0.37 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB2 | 1 | 0.37 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB3 | 1 | 0.37 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB1 | 1 | 0.37 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB2 | 1 | 0.37 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB3 | 1 | 0.37 |
| (1,2998) | 1:59:A:TYR:HB3 | 1:140:A:ALA:HB1 | 15 | 0.37 |
| (1,2998) | 1:59:A:TYR:HB3 | 1:140:A:ALA:HB2 | 15 | 0.37 |
| (1,2998) | 1:59:A:TYR:HB3 | 1:140:A:ALA:HB3 | 15 | 0.37 |
| (1,2943) | 1:3:A:ILE:HG21 | 1:8:A:GLN:HG3 | 7 | 0.37 |
| (1,2943) | 1:3:A:ILE:HG22 | 1:8:A:GLN:HG3 | 7 | 0.37 |
| (1,2943) | 1:3:A:ILE:HG23 | 1:8:A:GLN:HG3 | 7 | 0.37 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG11 | 11 | 0.37 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG12 | 11 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG13 | 11 | 0.37 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG11 | 11 | 0.37 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG12 | 11 | 0.37 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG13 | 11 | 0.37 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG11 | 11 | 0.37 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG12 | 11 | 0.37 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG13 | 11 | 0.37 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 4 | 0.37 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 4 | 0.37 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 4 | 0.37 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 3 | 0.37 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 10 | 0.37 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 19 | 0.37 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 2 | 0.37 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 2 | 0.37 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 2 | 0.37 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 12 | 0.37 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 12 | 0.37 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 12 | 0.37 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 17 | 0.37 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 17 | 0.37 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 17 | 0.37 |
| (1,2756) | 1:146:A:LEU:HA | 1:147:A:GLN:H | 3 | 0.37 |
| (1,2756) | 1:146:A:LEU:HA | 1:147:A:GLN:H | 5 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 13 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 13 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 13 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 13 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 13 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 13 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 18 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 18 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 18 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 18 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 18 | 0.37 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 18 | 0.37 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 8 | 0.37 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 8 | 0.37 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 8 | 0.37 |
| (1,2699) | 1:134:A:VAL:HG11 | 1:138:A:GLU:HG3 | 13 | 0.37 |
| (1,2699) | 1:134:A:VAL:HG12 | 1:138:A:GLU:HG3 | 13 | 0.37 |
| (1,2699) | 1:134:A:VAL:HG13 | 1:138:A:GLU:HG3 | 13 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 15 | 0.37 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 15 | 0.37 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 15 | 0.37 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 20 | 0.37 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 20 | 0.37 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 20 | 0.37 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 8 | 0.37 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 8 | 0.37 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 8 | 0.37 |
| (1,2581) | 1:52:A:GLU:HA | 1:53:A:GLY:HA3 | 5 | 0.37 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 19 | 0.37 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 19 | 0.37 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 19 | 0.37 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 19 | 0.37 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 19 | 0.37 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 19 | 0.37 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 19 | 0.37 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 19 | 0.37 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 19 | 0.37 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG21 | 11 | 0.37 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG22 | 11 | 0.37 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG23 | 11 | 0.37 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG21 | 11 | 0.37 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG22 | 11 | 0.37 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG23 | 11 | 0.37 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG21 | 11 | 0.37 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG22 | 11 | 0.37 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG23 | 11 | 0.37 |
| (1,2491) | 1:176:A:GLN:HA | 1:176:A:GLN:HE22 | 14 | 0.37 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 12 | 0.37 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 12 | 0.37 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 12 | 0.37 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 12 | 0.37 |
| (1,2304) | 1:132:A:SER:HA | 1:136:A:GLN:HG2 | 14 | 0.37 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 11 | 0.37 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 16 | 0.37 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 20 | 0.37 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 13 | 0.37 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 19 | 0.37 |
| (1,2070) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD3 | 19 | 0.37 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 8 | 0.37 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD1 | 6 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD2 | 6 | 0.37 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG11 | 16 | 0.37 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG12 | 16 | 0.37 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG13 | 16 | 0.37 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 12 | 0.37 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 6 | 0.37 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 4 | 0.37 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 12 | 0.37 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 5 | 0.37 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 16 | 0.37 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 19 | 0.37 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 19 | 0.37 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 19 | 0.37 |
| (1,1873) | 1:46:A:VAL:HA | 1:49:A:LYS:HB3 | 13 | 0.37 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 15 | 0.37 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 16 | 0.37 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 20 | 0.37 |
| (1,1694) | 1:136:A:GLN:HG2 | 1:137:A:GLN:H | 10 | 0.37 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 2 | 0.37 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 2 | 0.37 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 2 | 0.37 |
| (1,1604) | 1:61:A:VAL:HA | 1:62:A:GLU:HG2 | 12 | 0.37 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 11 | 0.37 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 1 | 0.37 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 12 | 0.37 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 10 | 0.37 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 10 | 0.37 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 10 | 0.37 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 20 | 0.37 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 20 | 0.37 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 20 | 0.37 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 8 | 0.37 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 8 | 0.37 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 8 | 0.37 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 16 | 0.37 |
| (1,1358) | 1:179:A:ASP:HB3 | 1:183:A:GLN:HE21 | 19 | 0.37 |
| (1,1258) | 1:163:A:GLN:HG2 | 1:164:A:GLY:HA3 | 16 | 0.37 |
| (1,1258) | 1:163:A:GLN:HG3 | 1:164:A:GLY:HA3 | 16 | 0.37 |
| (1,1164) | 1:27:A:SER:H | 1:30:A:CYS:HB3 | 12 | 0.37 |
| (1,898) | 1:103:A:SER:H | 1:107:A:ILE:HG13 | 13 | 0.37 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 7 | 0.37 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 7 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 7 | 0.37 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 9 | 0.37 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 9 | 0.37 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 9 | 0.37 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 7 | 0.37 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 3 | 0.37 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 3 | 0.37 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 3 | 0.37 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 18 | 0.37 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 18 | 0.37 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 18 | 0.37 |
| (1,726) | 1:161:A:ASN:H | 1:161:A:ASN:HD22 | 18 | 0.37 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 13 | 0.37 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 12 | 0.37 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 12 | 0.37 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 12 | 0.37 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 1 | 0.37 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 1 | 0.37 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 1 | 0.37 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 13 | 0.37 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 13 | 0.37 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 13 | 0.37 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 17 | 0.37 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 17 | 0.37 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 17 | 0.37 |
| (1,498) | 1:77:A:VAL:HG11 | 1:124:A:ALA:H | 7 | 0.37 |
| (1,498) | 1:77:A:VAL:HG12 | 1:124:A:ALA:H | 7 | 0.37 |
| (1,498) | 1:77:A:VAL:HG13 | 1:124:A:ALA:H | 7 | 0.37 |
| (1,485) | 1:4:A:THR:H | 1:7:A:LYS:HB2 | 7 | 0.37 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 16 | 0.37 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 16 | 0.37 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 16 | 0.37 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 17 | 0.37 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 17 | 0.37 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 17 | 0.37 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 17 | 0.37 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 20 | 0.37 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 3 | 0.37 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 3 | 0.37 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 3 | 0.37 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 10 | 0.37 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 10 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 10 | 0.37 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 19 | 0.37 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 19 | 0.37 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 19 | 0.37 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 5 | 0.37 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 5 | 0.37 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 5 | 0.37 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 20 | 0.37 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 20 | 0.37 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 20 | 0.37 |
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 3 | 0.37 |
| (1,241) | 1:70:A:ASP:HB2 | 1:74:A:ALA:H | 7 | 0.37 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 19 | 0.37 |
| (1,185) | 1:59:A:TYR:HB2 | 1:60:A:HIS:H | 7 | 0.37 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 15 | 0.37 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 15 | 0.37 |
| (1,132) | 1:56:A:MET:HB2 | 1:57:A:THR:H | 17 | 0.37 |
| (1,127) | 1:105:A:ALA:H | 1:107:A:ILE:HB | 16 | 0.37 |
| (1,127) | 1:105:A:ALA:H | 1:107:A:ILE:HB | 17 | 0.37 |
| (1,118) | 1:159:A:GLN:H | 1:184:A:LEU:HD21 | 8 | 0.37 |
| (1,118) | 1:159:A:GLN:H | 1:184:A:LEU:HD22 | 8 | 0.37 |
| (1,118) | 1:159:A:GLN:H | 1:184:A:LEU:HD23 | 8 | 0.37 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 11 | 0.37 |
| (1,78) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 15 | 0.37 |
| (1,67) | 1:26:A:PHE:H | 1:59:A:TYR:H | 16 | 0.37 |
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 12 | 0.37 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 12 | 0.36 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 12 | 0.36 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 12 | 0.36 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 12 | 0.36 |
| (1,3481) | 1:29:A:TYR:HE1 | 1:67:A:LEU:HA | 7 | 0.36 |
| (1,3481) | 1:29:A:TYR:HE2 | 1:67:A:LEU:HA | 7 | 0.36 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 16 | 0.36 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 16 | 0.36 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 9 | 0.36 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 9 | 0.36 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 8 | 0.36 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 8 | 0.36 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 5 | 0.36 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 5 | 0.36 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 19 | 0.36 |
| (1,3311) | 1:29:A:TYR:HD1 | 1:71:A:LEU:HB2 | 15 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3311) | 1:29:A:TYR:HD2 | 1:71:A:LEU:HB2 | 15 | 0.36 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 14 | 0.36 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 14 | 0.36 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 14 | 0.36 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 14 | 0.36 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 14 | 0.36 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 14 | 0.36 |
| (1,3295) | 1:30:A:CYS:HB3 | 1:34:A:TYR:H | 7 | 0.36 |
| (1,3112) | 1:67:A:LEU:HA | 1:70:A:ASP:HB3 | 20 | 0.36 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG21 | 17 | 0.36 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG22 | 17 | 0.36 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG23 | 17 | 0.36 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG21 | 17 | 0.36 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG22 | 17 | 0.36 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG23 | 17 | 0.36 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG21 | 17 | 0.36 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG22 | 17 | 0.36 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG23 | 17 | 0.36 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB1 | 3 | 0.36 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB2 | 3 | 0.36 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB3 | 3 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD21 | 16 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD22 | 16 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD23 | 16 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD21 | 16 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD22 | 16 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD23 | 16 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD21 | 16 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD22 | 16 | 0.36 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD23 | 16 | 0.36 |
| (1,2945) | 1:23:A:LEU:HD21 | 1:58:A:LYS:HA | 9 | 0.36 |
| (1,2945) | 1:23:A:LEU:HD22 | 1:58:A:LYS:HA | 9 | 0.36 |
| (1,2945) | 1:23:A:LEU:HD23 | 1:58:A:LYS:HA | 9 | 0.36 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 17 | 0.36 |
| (1,2832) | 1:55:A:LYS:HA | 1:56:A:MET:HB2 | 14 | 0.36 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 7 | 0.36 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 7 | 0.36 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 7 | 0.36 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 7 | 0.36 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 7 | 0.36 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 7 | 0.36 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 7 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 7 | 0.36 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 7 | 0.36 |
| (1,2756) | 1:146:A:LEU:HA | 1:147:A:GLN:H | 2 | 0.36 |
| (1,2756) | 1:146:A:LEU:HA | 1:147:A:GLN:H | 16 | 0.36 |
| (1,2756) | 1:146:A:LEU:HA | 1:147:A:GLN:H | 20 | 0.36 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 9 | 0.36 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 9 | 0.36 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 9 | 0.36 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 4 | 0.36 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 4 | 0.36 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 4 | 0.36 |
| (1,2581) | 1:52:A:GLU:HA | 1:53:A:GLY:HA3 | 8 | 0.36 |
| (1,2518) | 1:108:A:ARG:HA | 1:108:A:ARG:HG3 | 9 | 0.36 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG21 | 14 | 0.36 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG22 | 14 | 0.36 |
| (1,2460) | 1:73:A:GLN:HB3 | 1:134:A:VAL:HG23 | 14 | 0.36 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 17 | 0.36 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 17 | 0.36 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 17 | 0.36 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 2 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 2 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 2 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 2 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 2 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 2 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 2 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 5 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 5 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 5 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 5 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 5 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 5 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 20 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 20 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 20 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 20 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 20 | 0.36 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 20 | 0.36 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 13 | 0.36 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG21 | 2 | 0.36 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG22 | 2 | 0.36 |
| (1,2138) | 1:71:A:LEU:HD11 | 1:95:A:VAL:HG23 | 2 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG21 | 2 | 0.36 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG22 | 2 | 0.36 |
| (1,2138) | 1:71:A:LEU:HD12 | 1:95:A:VAL:HG23 | 2 | 0.36 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG21 | 2 | 0.36 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG22 | 2 | 0.36 |
| (1,2138) | 1:71:A:LEU:HD13 | 1:95:A:VAL:HG23 | 2 | 0.36 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 4 | 0.36 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 13 | 0.36 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 5 | 0.36 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 10 | 0.36 |
| (1,2016) | 1:117:A:LYS:HD3 | 1:119:A:GLU:H | 20 | 0.36 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 2 | 0.36 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 4 | 0.36 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 19 | 0.36 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 2 | 0.36 |
| (1,1935) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HA | 9 | 0.36 |
| (1,1695) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HE22 | 16 | 0.36 |
| (1,1694) | 1:136:A:GLN:HG2 | 1:137:A:GLN:H | 14 | 0.36 |
| (1,1686) | 1:99:A:GLN:HG3 | 1:100:A:THR:H | 17 | 0.36 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 16 | 0.36 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 16 | 0.36 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 16 | 0.36 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 16 | 0.36 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 17 | 0.36 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 17 | 0.36 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 17 | 0.36 |
| (1,1606) | 1:52:A:GLU:HG2 | 1:53:A:GLY:HA3 | 6 | 0.36 |
| (1,1606) | 1:52:A:GLU:HG3 | 1:53:A:GLY:HA3 | 6 | 0.36 |
| (1,1604) | 1:61:A:VAL:HA | 1:62:A:GLU:HG2 | 17 | 0.36 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 15 | 0.36 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 20 | 0.36 |
| (1,1565) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 1 | 0.36 |
| (1,1565) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 13 | 0.36 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 10 | 0.36 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 10 | 0.36 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 10 | 0.36 |
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 13 | 0.36 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 13 | 0.36 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 13 | 0.36 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 9 | 0.36 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 9 | 0.36 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 9 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG11 | 3 | 0.36 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG12 | 3 | 0.36 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG13 | 3 | 0.36 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 3 | 0.36 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 3 | 0.36 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 3 | 0.36 |
| (1,1427) | 1:143:A:ASP:HB2 | 1:145:A:GLN:HE22 | 2 | 0.36 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 9 | 0.36 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 13 | 0.36 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 17 | 0.36 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB2 | 10 | 0.36 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB3 | 10 | 0.36 |
| (1,1294) | 1:71:A:LEU:HB2 | 1:74:A:ALA:H | 11 | 0.36 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 5 | 0.36 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 16 | 0.36 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 19 | 0.36 |
| (1,1191) | 1:64:A:LEU:HD11 | 1:65:A:GLY:H | 4 | 0.36 |
| (1,1191) | 1:64:A:LEU:HD12 | 1:65:A:GLY:H | 4 | 0.36 |
| (1,1191) | 1:64:A:LEU:HD13 | 1:65:A:GLY:H | 4 | 0.36 |
| (1,1005) | 1:46:A:VAL:HG21 | 1:48:A:GLN:H | 8 | 0.36 |
| (1,1005) | 1:46:A:VAL:HG22 | 1:48:A:GLN:H | 8 | 0.36 |
| (1,1005) | 1:46:A:VAL:HG23 | 1:48:A:GLN:H | 8 | 0.36 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 8 | 0.36 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 10 | 0.36 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 17 | 0.36 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 3 | 0.36 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 4 | 0.36 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 10 | 0.36 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 10 | 0.36 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 10 | 0.36 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 5 | 0.36 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 5 | 0.36 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 5 | 0.36 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 3 | 0.36 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 3 | 0.36 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 3 | 0.36 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 10 | 0.36 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 10 | 0.36 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 10 | 0.36 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 13 | 0.36 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 13 | 0.36 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 13 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 20 | 0.36 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 20 | 0.36 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 20 | 0.36 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 10 | 0.36 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 1 | 0.36 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 1 | 0.36 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 1 | 0.36 |
| (1,683) | 1:168:A:SER:H | 1:170:A:MET:HG2 | 16 | 0.36 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 4 | 0.36 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 20 | 0.36 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 20 | 0.36 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 20 | 0.36 |
| (1,259) | 1:69:A:LYS:HD2 | 1:70:A:ASP:H | 8 | 0.36 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 17 | 0.36 |
| (1,127) | 1:105:A:ALA:H | 1:107:A:ILE:HB | 3 | 0.36 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 8 | 0.36 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 20 | 0.36 |
| (1,67) | 1:26:A:PHE:H | 1:59:A:TYR:H | 13 | 0.36 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 14 | 0.36 |
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 4 | 0.36 |
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 16 | 0.36 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 17 | 0.35 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 17 | 0.35 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 17 | 0.35 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 17 | 0.35 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 17 | 0.35 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 17 | 0.35 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB2 | 19 | 0.35 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB3 | 19 | 0.35 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB2 | 19 | 0.35 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB3 | 19 | 0.35 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 8 | 0.35 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 15 | 0.35 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 15 | 0.35 |
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 15 | 0.35 |
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 15 | 0.35 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 3 | 0.35 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 3 | 0.35 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 3 | 0.35 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 3 | 0.35 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 3 | 0.35 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 3 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 9 | 0.35 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 9 | 0.35 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 9 | 0.35 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 9 | 0.35 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 9 | 0.35 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 9 | 0.35 |
| (1,3297) | 1:23:A:LEU:HB2 | 1:153:A:TYR:H | 7 | 0.35 |
| (1,3269) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA2 | 20 | 0.35 |
| (1,3269) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA2 | 20 | 0.35 |
| (1,3269) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA2 | 20 | 0.35 |
| (1,3252) | 1:29:A:TYR:HD1 | 1:68:A:GLY:HA3 | 1 | 0.35 |
| (1,3252) | 1:29:A:TYR:HD2 | 1:68:A:GLY:HA3 | 1 | 0.35 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 12 | 0.35 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 12 | 0.35 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 12 | 0.35 |
| (1,3112) | 1:67:A:LEU:HA | 1:70:A:ASP:HB3 | 19 | 0.35 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG21 | 18 | 0.35 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG22 | 18 | 0.35 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG23 | 18 | 0.35 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG21 | 18 | 0.35 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG22 | 18 | 0.35 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG23 | 18 | 0.35 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG21 | 18 | 0.35 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG22 | 18 | 0.35 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG23 | 18 | 0.35 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD21 | 1 | 0.35 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD22 | 1 | 0.35 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD23 | 1 | 0.35 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG11 | 18 | 0.35 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG12 | 18 | 0.35 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG13 | 18 | 0.35 |
| (1,2943) | 1:3:A:ILE:HG21 | 1:8:A:GLN:HG3 | 11 | 0.35 |
| (1,2943) | 1:3:A:ILE:HG22 | 1:8:A:GLN:HG3 | 11 | 0.35 |
| (1,2943) | 1:3:A:ILE:HG23 | 1:8:A:GLN:HG3 | 11 | 0.35 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 13 | 0.35 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD11 | 1 | 0.35 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD12 | 1 | 0.35 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD13 | 1 | 0.35 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 20 | 0.35 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 20 | 0.35 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 20 | 0.35 |
| (1,2756) | 1:146:A:LEU:HA | 1:147:A:GLN:H | 12 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2756) | 1:146:A:LEU:HA | 1:147:A:GLN:H | 17 | 0.35 |
| (1,2452) | 1:149:A:VAL:HG11 | 1:150:A:PRO:HG3 | 3 | 0.35 |
| (1,2452) | 1:149:A:VAL:HG12 | 1:150:A:PRO:HG3 | 3 | 0.35 |
| (1,2452) | 1:149:A:VAL:HG13 | 1:150:A:PRO:HG3 | 3 | 0.35 |
| (1,2452) | 1:149:A:VAL:HG21 | 1:150:A:PRO:HG3 | 3 | 0.35 |
| (1,2452) | 1:149:A:VAL:HG22 | 1:150:A:PRO:HG3 | 3 | 0.35 |
| (1,2452) | 1:149:A:VAL:HG23 | 1:150:A:PRO:HG3 | 3 | 0.35 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE1 | 18 | 0.35 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE2 | 18 | 0.35 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE1 | 18 | 0.35 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE2 | 18 | 0.35 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE1 | 18 | 0.35 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE2 | 18 | 0.35 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 5 | 0.35 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 6 | 0.35 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 10 | 0.35 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 12 | 0.35 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 19 | 0.35 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG11 | 6 | 0.35 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG12 | 6 | 0.35 |
| (1,2196) | 1:108:A:ARG:HG3 | 1:112:A:VAL:HG13 | 6 | 0.35 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 17 | 0.35 |
| (1,2159) | 1:76:A:ALA:HA | 1:79:A:ILE:HG12 | 6 | 0.35 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 13 | 0.35 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 13 | 0.35 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 13 | 0.35 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 13 | 0.35 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 13 | 0.35 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 13 | 0.35 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG11 | 17 | 0.35 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG12 | 17 | 0.35 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG13 | 17 | 0.35 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 5 | 0.35 |
| (1,1981) | 1:187:A:LYS:H | 1:187:A:LYS:HD3 | 7 | 0.35 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 17 | 0.35 |
| (1,1931) | 1:62:A:GLU:HB2 | 1:63:A:PHE:HB3 | 12 | 0.35 |
| (1,1931) | 1:62:A:GLU:HB3 | 1:63:A:PHE:HB3 | 12 | 0.35 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 11 | 0.35 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 13 | 0.35 |
| (1,1813) | 1:160:A:LEU:HD21 | 1:180:A:THR:HB | 12 | 0.35 |
| (1,1813) | 1:160:A:LEU:HD22 | 1:180:A:THR:HB | 12 | 0.35 |
| (1,1813) | 1:160:A:LEU:HD23 | 1:180:A:THR:HB | 12 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 1 | 0.35 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD1 | 1 | 0.35 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD2 | 1 | 0.35 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 18 | 0.35 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 18 | 0.35 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 18 | 0.35 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 18 | 0.35 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 18 | 0.35 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 18 | 0.35 |
| (1,1698) | 1:136:A:GLN:HB2 | 1:136:A:GLN:HG2 | 10 | 0.35 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 18 | 0.35 |
| (1,1695) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HE22 | 17 | 0.35 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 5 | 0.35 |
| (1,1588) | 1:62:A:GLU:HA | 1:62:A:GLU:HG3 | 4 | 0.35 |
| (1,1573) | 1:119:A:GLU:HG2 | 1:120:A:ASP:HB2 | 19 | 0.35 |
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 3 | 0.35 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 3 | 0.35 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 3 | 0.35 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 16 | 0.35 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 16 | 0.35 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 16 | 0.35 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 13 | 0.35 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 13 | 0.35 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 13 | 0.35 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG11 | 14 | 0.35 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG12 | 14 | 0.35 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG13 | 14 | 0.35 |
| (1,1474) | 1:161:A:ASN:HB2 | 1:161:A:ASN:HD22 | 5 | 0.35 |
| (1,1445) | 1:116:A:VAL:HG21 | 1:120:A:ASP:HB3 | 1 | 0.35 |
| (1,1445) | 1:116:A:VAL:HG22 | 1:120:A:ASP:HB3 | 1 | 0.35 |
| (1,1445) | 1:116:A:VAL:HG23 | 1:120:A:ASP:HB3 | 1 | 0.35 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 2 | 0.35 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 2 | 0.35 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 2 | 0.35 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB2 | 11 | 0.35 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB3 | 11 | 0.35 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 4 | 0.35 |
| (1,1258) | 1:163:A:GLN:HG2 | 1:164:A:GLY:HA3 | 2 | 0.35 |
| (1,1258) | 1:163:A:GLN:HG3 | 1:164:A:GLY:HA3 | 2 | 0.35 |
| (1,1258) | 1:163:A:GLN:HG2 | 1:164:A:GLY:HA3 | 14 | 0.35 |
| (1,1258) | 1:163:A:GLN:HG3 | 1:164:A:GLY:HA3 | 14 | 0.35 |
| (1,1258) | 1:163:A:GLN:HG2 | 1:164:A:GLY:HA3 | 20 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1258) | 1:163:A:GLN:HG3 | 1:164:A:GLY:HA3 | 20 | 0.35 |
| (1,1164) | 1:27:A:SER:H | 1:30:A:CYS:HB3 | 6 | 0.35 |
| (1,1164) | 1:27:A:SER:H | 1:30:A:CYS:HB3 | 10 | 0.35 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 6 | 0.35 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG21 | 11 | 0.35 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG22 | 11 | 0.35 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG23 | 11 | 0.35 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 1 | 0.35 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 1 | 0.35 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 1 | 0.35 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 8 | 0.35 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 20 | 0.35 |
| (1,606) | 1:137:A:GLN:H | 1:137:A:GLN:HG2 | 14 | 0.35 |
| (1,606) | 1:137:A:GLN:H | 1:137:A:GLN:HG2 | 18 | 0.35 |
| (1,555) | 1:174:A:VAL:HG21 | 1:178:A:ALA:H | 18 | 0.35 |
| (1,555) | 1:174:A:VAL:HG22 | 1:178:A:ALA:H | 18 | 0.35 |
| (1,555) | 1:174:A:VAL:HG23 | 1:178:A:ALA:H | 18 | 0.35 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 16 | 0.35 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 5 | 0.35 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 5 | 0.35 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 5 | 0.35 |
| (1,498) | 1:77:A:VAL:HG11 | 1:124:A:ALA:H | 19 | 0.35 |
| (1,498) | 1:77:A:VAL:HG12 | 1:124:A:ALA:H | 19 | 0.35 |
| (1,498) | 1:77:A:VAL:HG13 | 1:124:A:ALA:H | 19 | 0.35 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 10 | 0.35 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 10 | 0.35 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 10 | 0.35 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 13 | 0.35 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 13 | 0.35 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 13 | 0.35 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 14 | 0.35 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 14 | 0.35 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 14 | 0.35 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 19 | 0.35 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 19 | 0.35 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 19 | 0.35 |
| (1,438) | 1:60:A:HIS:HB2 | 1:75:A:TRP:H | 17 | 0.35 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 1 | 0.35 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 1 | 0.35 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 1 | 0.35 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 4 | 0.35 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 4 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 4 | 0.35 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 6 | 0.35 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 6 | 0.35 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 6 | 0.35 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 8 | 0.35 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 8 | 0.35 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 8 | 0.35 |
| (1,259) | 1:69:A:LYS:HD2 | 1:70:A:ASP:H | 1 | 0.35 |
| (1,259) | 1:69:A:LYS:HD2 | 1:70:A:ASP:H | 20 | 0.35 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 11 | 0.35 |
| (1,128) | 1:12:A:LEU:HD11 | 1:159:A:GLN:H | 13 | 0.35 |
| (1,128) | 1:12:A:LEU:HD12 | 1:159:A:GLN:H | 13 | 0.35 |
| (1,128) | 1:12:A:LEU:HD13 | 1:159:A:GLN:H | 13 | 0.35 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 3 | 0.35 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 6 | 0.35 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 12 | 0.35 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG21 | 10 | 0.35 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG22 | 10 | 0.35 |
| (1,41) | 1:5:A:ASP:H | 1:11:A:THR:HG23 | 10 | 0.35 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 5 | 0.34 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 5 | 0.34 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 5 | 0.34 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 5 | 0.34 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 5 | 0.34 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 5 | 0.34 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 10 | 0.34 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 1 | 0.34 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 1 | 0.34 |
| (1,3474) | 1:153:A:TYR:HE1 | 1:160:A:LEU:H | 1 | 0.34 |
| (1,3474) | 1:153:A:TYR:HE2 | 1:160:A:LEU:H | 1 | 0.34 |
| (1,3345) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 16 | 0.34 |
| (1,3345) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 16 | 0.34 |
| (1,3345) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 16 | 0.34 |
| (1,3345) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 16 | 0.34 |
| (1,3345) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 16 | 0.34 |
| (1,3345) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 16 | 0.34 |
| (1,3345) | 1:46:A:VAL:HG21 | 1:177:A:TYR:HD1 | 16 | 0.34 |
| (1,3345) | 1:46:A:VAL:HG21 | 1:177:A:TYR:HD2 | 16 | 0.34 |
| (1,3345) | 1:46:A:VAL:HG22 | 1:177:A:TYR:HD1 | 16 | 0.34 |
| (1,3345) | 1:46:A:VAL:HG22 | 1:177:A:TYR:HD2 | 16 | 0.34 |
| (1,3345) | 1:46:A:VAL:HG23 | 1:177:A:TYR:HD1 | 16 | 0.34 |
| (1,3345) | 1:46:A:VAL:HG23 | 1:177:A:TYR:HD2 | 16 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 6 | 0.34 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 6 | 0.34 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 6 | 0.34 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 6 | 0.34 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 6 | 0.34 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 6 | 0.34 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG11 | 2 | 0.34 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG12 | 2 | 0.34 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG13 | 2 | 0.34 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 10 | 0.34 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 10 | 0.34 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 10 | 0.34 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 10 | 0.34 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 10 | 0.34 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 10 | 0.34 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 10 | 0.34 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 10 | 0.34 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 10 | 0.34 |
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 3 | 0.34 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 12 | 0.34 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 12 | 0.34 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 12 | 0.34 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 11 | 0.34 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 14 | 0.34 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB1 | 18 | 0.34 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB2 | 18 | 0.34 |
| (1,2894) | 1:0:A:ASN:HA | 1:1:A:ALA:HB3 | 18 | 0.34 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 19 | 0.34 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 19 | 0.34 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 19 | 0.34 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 20 | 0.34 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 20 | 0.34 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 20 | 0.34 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 2 | 0.34 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 2 | 0.34 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 2 | 0.34 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 6 | 0.34 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 6 | 0.34 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 6 | 0.34 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 10 | 0.34 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 10 | 0.34 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 10 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2693) | 1:117:A:LYS:HA | 1:117:A:LYS:HG3 | 7 | 0.34 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG21 | 11 | 0.34 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG22 | 11 | 0.34 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG23 | 11 | 0.34 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG21 | 11 | 0.34 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG22 | 11 | 0.34 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG23 | 11 | 0.34 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG21 | 11 | 0.34 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG22 | 11 | 0.34 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG23 | 11 | 0.34 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 8 | 0.34 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 8 | 0.34 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 8 | 0.34 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 9 | 0.34 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 9 | 0.34 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 9 | 0.34 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 9 | 0.34 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 9 | 0.34 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 9 | 0.34 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 9 | 0.34 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 9 | 0.34 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 9 | 0.34 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG21 | 2 | 0.34 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG22 | 2 | 0.34 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG23 | 2 | 0.34 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 9 | 0.34 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 9 | 0.34 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 9 | 0.34 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 3 | 0.34 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 4 | 0.34 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 6 | 0.34 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 6 | 0.34 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 6 | 0.34 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 6 | 0.34 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 6 | 0.34 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 6 | 0.34 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 6 | 0.34 |
| (1,2159) | 1:76:A:ALA:HA | 1:79:A:ILE:HG12 | 15 | 0.34 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 17 | 0.34 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 17 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG21 | 1 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG22 | 1 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG23 | 1 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG21 | 1 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG22 | 1 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG23 | 1 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG21 | 4 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG22 | 4 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG23 | 4 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG21 | 4 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG22 | 4 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG23 | 4 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG21 | 17 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG22 | 17 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG23 | 17 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG21 | 17 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG22 | 17 | 0.34 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG23 | 17 | 0.34 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG11 | 10 | 0.34 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG12 | 10 | 0.34 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG13 | 10 | 0.34 |
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 4 | 0.34 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 8 | 0.34 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 8 | 0.34 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 8 | 0.34 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 8 | 0.34 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 10 | 0.34 |
| (1,1813) | 1:160:A:LEU:HD21 | 1:180:A:THR:HB | 3 | 0.34 |
| (1,1813) | 1:160:A:LEU:HD22 | 1:180:A:THR:HB | 3 | 0.34 |
| (1,1813) | 1:160:A:LEU:HD23 | 1:180:A:THR:HB | 3 | 0.34 |
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 1 | 0.34 |
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 1 | 0.34 |
| (1,1698) | 1:136:A:GLN:HB2 | 1:136:A:GLN:HG2 | 8 | 0.34 |
| (1,1698) | 1:136:A:GLN:HB2 | 1:136:A:GLN:HG2 | 15 | 0.34 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 13 | 0.34 |
| (1,1695) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HE22 | 3 | 0.34 |
| (1,1694) | 1:136:A:GLN:HG2 | 1:137:A:GLN:H | 8 | 0.34 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG2 | 4 | 0.34 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG3 | 4 | 0.34 |
| (1,1686) | 1:99:A:GLN:HG3 | 1:100:A:THR:H | 9 | 0.34 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 18 | 0.34 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 1 | 0.34 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 17 | 0.34 |
| (1,1588) | 1:62:A:GLU:HA | 1:62:A:GLU:HG3 | 7 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1588) | 1:62:A:GLU:HA | 1:62:A:GLU:HG3 | 9 | 0.34 |
| (1,1588) | 1:62:A:GLU:HA | 1:62:A:GLU:HG3 | 16 | 0.34 |
| (1,1563) | 1:152:A:MET:HB3 | 1:160:A:LEU:HB3 | 2 | 0.34 |
| (1,1563) | 1:152:A:MET:HB3 | 1:160:A:LEU:HB3 | 12 | 0.34 |
| (1,1563) | 1:152:A:MET:HB3 | 1:160:A:LEU:HB3 | 15 | 0.34 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG11 | 7 | 0.34 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG12 | 7 | 0.34 |
| (1,1557) | 1:152:A:MET:HB2 | 1:181:A:VAL:HG13 | 7 | 0.34 |
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 10 | 0.34 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 10 | 0.34 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 10 | 0.34 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 2 | 0.34 |
| (1,1526) | 1:63:A:PHE:HB2 | 1:64:A:LEU:H | 14 | 0.34 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 15 | 0.34 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 15 | 0.34 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 15 | 0.34 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 2 | 0.34 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 2 | 0.34 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 2 | 0.34 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 15 | 0.34 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 15 | 0.34 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 15 | 0.34 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE2 | 19 | 0.34 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE3 | 19 | 0.34 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE2 | 19 | 0.34 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE3 | 19 | 0.34 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE2 | 19 | 0.34 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE3 | 19 | 0.34 |
| (1,1255) | 1:6:A:GLY:HA2 | 1:7:A:LYS:HB3 | 7 | 0.34 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 4 | 0.34 |
| (1,1185) | 1:29:A:TYR:HE1 | 1:68:A:GLY:H | 19 | 0.34 |
| (1,1185) | 1:29:A:TYR:HE2 | 1:68:A:GLY:H | 19 | 0.34 |
| (1,1164) | 1:27:A:SER:H | 1:30:A:CYS:HB3 | 15 | 0.34 |
| (1,1116) | 1:61:A:VAL:HG11 | 1:63:A:PHE:H | 18 | 0.34 |
| (1,1116) | 1:61:A:VAL:HG12 | 1:63:A:PHE:H | 18 | 0.34 |
| (1,1116) | 1:61:A:VAL:HG13 | 1:63:A:PHE:H | 18 | 0.34 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 12 | 0.34 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 16 | 0.34 |
| (1,1040) | 1:52:A:GLU:HB3 | 1:53:A:GLY:H | 7 | 0.34 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG21 | 20 | 0.34 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG22 | 20 | 0.34 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG23 | 20 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 18 | 0.34 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 18 | 0.34 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 18 | 0.34 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG11 | 18 | 0.34 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG12 | 18 | 0.34 |
| (1,829) | 1:174:A:VAL:H | 1:174:A:VAL:HG13 | 18 | 0.34 |
| (1,763) | 1:103:A:SER:HB2 | 1:106:A:ASP:H | 6 | 0.34 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 14 | 0.34 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 15 | 0.34 |
| (1,587) | 1:46:A:VAL:HG21 | 1:47:A:ARG:H | 1 | 0.34 |
| (1,587) | 1:46:A:VAL:HG22 | 1:47:A:ARG:H | 1 | 0.34 |
| (1,587) | 1:46:A:VAL:HG23 | 1:47:A:ARG:H | 1 | 0.34 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 10 | 0.34 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 10 | 0.34 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 10 | 0.34 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 20 | 0.34 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 20 | 0.34 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 20 | 0.34 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 10 | 0.34 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 4 | 0.34 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 4 | 0.34 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 4 | 0.34 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 6 | 0.34 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 6 | 0.34 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 6 | 0.34 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 20 | 0.34 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 20 | 0.34 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 20 | 0.34 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 7 | 0.34 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 5 | 0.34 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 5 | 0.34 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 5 | 0.34 |
| (1,285) | 1:152:A:MET:H | 1:152:A:MET:HB3 | 15 | 0.34 |
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 17 | 0.34 |
| (1,259) | 1:69:A:LYS:HD2 | 1:70:A:ASP:H | 14 | 0.34 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 1 | 0.34 |
| (1,216) | 1:34:A:TYR:H | 1:96:A:GLN:HE21 | 17 | 0.34 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 10 | 0.34 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE1 | 2 | 0.33 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE2 | 2 | 0.33 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE1 | 2 | 0.33 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE2 | 2 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE1 | 2 | 0.33 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE2 | 2 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 6 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 6 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 6 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 6 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 6 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 6 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 12 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 12 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 12 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 12 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 12 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 12 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 19 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 19 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 19 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 19 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 19 | 0.33 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 19 | 0.33 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 14 | 0.33 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 14 | 0.33 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 3 | 0.33 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 3 | 0.33 |
| (1,3420) | 1:60:A:HIS:HB3 | 1:75:A:TRP:HD1 | 3 | 0.33 |
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 3 | 0.33 |
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 3 | 0.33 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD11 | 20 | 0.33 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD12 | 20 | 0.33 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD13 | 20 | 0.33 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD11 | 20 | 0.33 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD12 | 20 | 0.33 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD13 | 20 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 7 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 7 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 7 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 7 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 7 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 7 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG21 | 1:177:A:TYR:HD1 | 7 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG21 | 1:177:A:TYR:HD2 | 7 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG22 | 1:177:A:TYR:HD1 | 7 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3345) | 1:46:A:VAL:HG22 | 1:177:A:TYR:HD2 | 7 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG23 | 1:177:A:TYR:HD1 | 7 | 0.33 |
| (1,3345) | 1:46:A:VAL:HG23 | 1:177:A:TYR:HD2 | 7 | 0.33 |
| (1,3311) | 1:29:A:TYR:HD1 | 1:71:A:LEU:HB2 | 9 | 0.33 |
| (1,3311) | 1:29:A:TYR:HD2 | 1:71:A:LEU:HB2 | 9 | 0.33 |
| (1,3250) | 1:68:A:GLY:HA3 | 1:71:A:LEU:HB2 | 4 | 0.33 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 16 | 0.33 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 16 | 0.33 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 16 | 0.33 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 16 | 0.33 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 16 | 0.33 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 16 | 0.33 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 16 | 0.33 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 16 | 0.33 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 16 | 0.33 |
| (1,3112) | 1:67:A:LEU:HA | 1:70:A:ASP:HB3 | 17 | 0.33 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 12 | 0.33 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 12 | 0.33 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 12 | 0.33 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 19 | 0.33 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 19 | 0.33 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 19 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG21 | 4 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG22 | 4 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG23 | 4 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG21 | 4 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG22 | 4 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG23 | 4 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG21 | 4 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG22 | 4 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG23 | 4 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG21 | 19 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG22 | 19 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG23 | 19 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG21 | 19 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG22 | 19 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG23 | 19 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG21 | 19 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG22 | 19 | 0.33 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG23 | 19 | 0.33 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG11 | 17 | 0.33 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG12 | 17 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG13 | 17 | 0.33 |
| (1,2935) | 1:75:A:TRP:HA | 1:78:A:ALA:HA | 5 | 0.33 |
| (1,2935) | 1:75:A:TRP:HA | 1:78:A:ALA:HA | 17 | 0.33 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 6 | 0.33 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 6 | 0.33 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 6 | 0.33 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 17 | 0.33 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 17 | 0.33 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 17 | 0.33 |
| (1,2756) | 1:146:A:LEU:HA | 1:147:A:GLN:H | 4 | 0.33 |
| (1,2756) | 1:146:A:LEU:HA | 1:147:A:GLN:H | 13 | 0.33 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG11 | 9 | 0.33 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG12 | 9 | 0.33 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG13 | 9 | 0.33 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 11 | 0.33 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 11 | 0.33 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 11 | 0.33 |
| (1,2632) | 1:101:A:VAL:HG21 | 1:107:A:ILE:H | 10 | 0.33 |
| (1,2632) | 1:101:A:VAL:HG22 | 1:107:A:ILE:H | 10 | 0.33 |
| (1,2632) | 1:101:A:VAL:HG23 | 1:107:A:ILE:H | 10 | 0.33 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 3 | 0.33 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 3 | 0.33 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 3 | 0.33 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 11 | 0.33 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 11 | 0.33 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 11 | 0.33 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 11 | 0.33 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 11 | 0.33 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 11 | 0.33 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 11 | 0.33 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 11 | 0.33 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 11 | 0.33 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 4 | 0.33 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 4 | 0.33 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 4 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 9 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 9 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 9 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 9 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 9 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 9 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 9 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 9 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 9 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 11 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 11 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 11 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 11 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 11 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 11 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 11 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 11 | 0.33 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 11 | 0.33 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 17 | 0.33 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 17 | 0.33 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 17 | 0.33 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 17 | 0.33 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 17 | 0.33 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 17 | 0.33 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 17 | 0.33 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 17 | 0.33 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 17 | 0.33 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 18 | 0.33 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 6 | 0.33 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 6 | 0.33 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 6 | 0.33 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 19 | 0.33 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 19 | 0.33 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 19 | 0.33 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 18 | 0.33 |
| (1,2316) | 1:117:A:LYS:H | 1:117:A:LYS:HG2 | 11 | 0.33 |
| (1,2315) | 1:46:A:VAL:HG21 | 1:50:A:LEU:HG | 15 | 0.33 |
| (1,2315) | 1:46:A:VAL:HG22 | 1:50:A:LEU:HG | 15 | 0.33 |
| (1,2315) | 1:46:A:VAL:HG23 | 1:50:A:LEU:HG | 15 | 0.33 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 3 | 0.33 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 3 | 0.33 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 3 | 0.33 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 3 | 0.33 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 3 | 0.33 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 3 | 0.33 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 9 | 0.33 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 14 | 0.33 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 2 | 0.33 |
| (1,2159) | 1:76:A:ALA:HA | 1:79:A:ILE:HG12 | 2 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2159) | 1:76:A:ALA:HA | 1:79:A:ILE:HG12 | 8 | 0.33 |
| (1,2118) | 1:10:A:ILE:HG13 | 1:159:A:GLN:H | 11 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG21 | 6 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG22 | 6 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG23 | 6 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG21 | 6 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG22 | 6 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG23 | 6 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG21 | 9 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG22 | 9 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG23 | 9 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG21 | 9 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG22 | 9 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG23 | 9 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG21 | 12 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG22 | 12 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG23 | 12 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG21 | 12 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG22 | 12 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG23 | 12 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG21 | 20 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG22 | 20 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG23 | 20 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG21 | 20 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG22 | 20 | 0.33 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG23 | 20 | 0.33 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 10 | 0.33 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 12 | 0.33 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 14 | 0.33 |
| (1,2016) | 1:117:A:LYS:HD3 | 1:119:A:GLU:H | 18 | 0.33 |
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 9 | 0.33 |
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 10 | 0.33 |
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 12 | 0.33 |
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 14 | 0.33 |
| (1,1988) | 1:136:A:GLN:H | 1:136:A:GLN:HB2 | 2 | 0.33 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 9 | 0.33 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 17 | 0.33 |
| (1,1931) | 1:62:A:GLU:HB2 | 1:63:A:PHE:HB3 | 8 | 0.33 |
| (1,1931) | 1:62:A:GLU:HB3 | 1:63:A:PHE:HB3 | 8 | 0.33 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG21 | 6 | 0.33 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG22 | 6 | 0.33 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG23 | 6 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 5 | 0.33 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 3 | 0.33 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 3 | 0.33 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 3 | 0.33 |
| (1,1782) | 1:46:A:VAL:HG21 | 1:56:A:MET:HG3 | 16 | 0.33 |
| (1,1782) | 1:46:A:VAL:HG22 | 1:56:A:MET:HG3 | 16 | 0.33 |
| (1,1782) | 1:46:A:VAL:HG23 | 1:56:A:MET:HG3 | 16 | 0.33 |
| (1,1778) | 1:72:A:THR:HB | 1:73:A:GLN:HB3 | 14 | 0.33 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 15 | 0.33 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 15 | 0.33 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 15 | 0.33 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 15 | 0.33 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 15 | 0.33 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 15 | 0.33 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG12 | 10 | 0.33 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG13 | 10 | 0.33 |
| (1,1698) | 1:136:A:GLN:HB2 | 1:136:A:GLN:HG2 | 3 | 0.33 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 17 | 0.33 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG2 | 15 | 0.33 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG3 | 15 | 0.33 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 4 | 0.33 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 6 | 0.33 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 15 | 0.33 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 19 | 0.33 |
| (1,1639) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG2 | 7 | 0.33 |
| (1,1639) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG2 | 7 | 0.33 |
| (1,1639) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG2 | 7 | 0.33 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 11 | 0.33 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 11 | 0.33 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 11 | 0.33 |
| (1,1606) | 1:52:A:GLU:HG2 | 1:53:A:GLY:HA3 | 16 | 0.33 |
| (1,1606) | 1:52:A:GLU:HG3 | 1:53:A:GLY:HA3 | 16 | 0.33 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 19 | 0.33 |
| (1,1565) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 10 | 0.33 |
| (1,1563) | 1:152:A:MET:HB3 | 1:160:A:LEU:HB3 | 1 | 0.33 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 20 | 0.33 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 20 | 0.33 |
| (1,1526) | 1:63:A:PHE:HB2 | 1:64:A:LEU:H | 1 | 0.33 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 5 | 0.33 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 5 | 0.33 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 5 | 0.33 |
| (1,1485) | 1:28:A:PHE:HB2 | 1:95:A:VAL:HB | 13 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1474) | 1:161:A:ASN:HB2 | 1:161:A:ASN:HD22 | 17 | 0.33 |
| (1,1432) | 1:85:A:ASP:HB3 | 1:86:A:LYS:HG2 | 14 | 0.33 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 8 | 0.33 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 8 | 0.33 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 8 | 0.33 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 1 | 0.33 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 10 | 0.33 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 20 | 0.33 |
| (1,1331) | 1:70:A:ASP:HB3 | 1:72:A:THR:H | 1 | 0.33 |
| (1,1331) | 1:70:A:ASP:HB3 | 1:72:A:THR:H | 5 | 0.33 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB2 | 15 | 0.33 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB3 | 15 | 0.33 |
| (1,1294) | 1:71:A:LEU:HB2 | 1:74:A:ALA:H | 20 | 0.33 |
| (1,1185) | 1:29:A:TYR:HE1 | 1:68:A:GLY:H | 8 | 0.33 |
| (1,1185) | 1:29:A:TYR:HE2 | 1:68:A:GLY:H | 8 | 0.33 |
| (1,1164) | 1:27:A:SER:H | 1:30:A:CYS:HB3 | 9 | 0.33 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 10 | 0.33 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 9 | 0.33 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 15 | 0.33 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 6 | 0.33 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 6 | 0.33 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 6 | 0.33 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 14 | 0.33 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 14 | 0.33 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 14 | 0.33 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 4 | 0.33 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 12 | 0.33 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 1 | 0.33 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 9 | 0.33 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 3 | 0.33 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 3 | 0.33 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 3 | 0.33 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 19 | 0.33 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 19 | 0.33 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 19 | 0.33 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 5 | 0.33 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 6 | 0.33 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 11 | 0.33 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 12 | 0.33 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 7 | 0.33 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 7 | 0.33 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 7 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 1 | 0.33 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 3 | 0.33 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 15 | 0.33 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 15 | 0.33 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 19 | 0.33 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 13 | 0.33 |
| (1,632) | 1:87:A:ILE:HG21 | 1:91:A:MET:H | 10 | 0.33 |
| (1,632) | 1:87:A:ILE:HG22 | 1:91:A:MET:H | 10 | 0.33 |
| (1,632) | 1:87:A:ILE:HG23 | 1:91:A:MET:H | 10 | 0.33 |
| (1,617) | 1:10:A:ILE:H | 1:159:A:GLN:HB2 | 5 | 0.33 |
| (1,560) | 1:42:A:VAL:HG21 | 1:178:A:ALA:H | 6 | 0.33 |
| (1,560) | 1:42:A:VAL:HG22 | 1:178:A:ALA:H | 6 | 0.33 |
| (1,560) | 1:42:A:VAL:HG23 | 1:178:A:ALA:H | 6 | 0.33 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 1 | 0.33 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 9 | 0.33 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 9 | 0.33 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 9 | 0.33 |
| (1,498) | 1:77:A:VAL:HG11 | 1:124:A:ALA:H | 17 | 0.33 |
| (1,498) | 1:77:A:VAL:HG12 | 1:124:A:ALA:H | 17 | 0.33 |
| (1,498) | 1:77:A:VAL:HG13 | 1:124:A:ALA:H | 17 | 0.33 |
| (1,485) | 1:4:A:THR:H | 1:7:A:LYS:HB2 | 9 | 0.33 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 9 | 0.33 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 9 | 0.33 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 9 | 0.33 |
| (1,405) | 1:25:A:PHE:H | 1:150:A:PRO:HB2 | 10 | 0.33 |
| (1,401) | 1:117:A:LYS:HB2 | 1:120:A:ASP:H | 16 | 0.33 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 13 | 0.33 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 13 | 0.33 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 13 | 0.33 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 17 | 0.33 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 17 | 0.33 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 17 | 0.33 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 18 | 0.33 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 18 | 0.33 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 18 | 0.33 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 3 | 0.33 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 3 | 0.33 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 3 | 0.33 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 14 | 0.33 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 14 | 0.33 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 14 | 0.33 |
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 10 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 16 | 0.33 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 2 | 0.33 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 9 | 0.33 |
| (1,216) | 1:34:A:TYR:H | 1:96:A:GLN:HE21 | 15 | 0.33 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 2 | 0.33 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 19 | 0.33 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 4 | 0.33 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 17 | 0.33 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE1 | 19 | 0.32 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE2 | 19 | 0.32 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE1 | 19 | 0.32 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE2 | 19 | 0.32 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE1 | 19 | 0.32 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE2 | 19 | 0.32 |
| (1,3495) | 1:23:A:LEU:HD21 | 1:59:A:TYR:HE1 | 5 | 0.32 |
| (1,3495) | 1:23:A:LEU:HD21 | 1:59:A:TYR:HE2 | 5 | 0.32 |
| (1,3495) | 1:23:A:LEU:HD22 | 1:59:A:TYR:HE1 | 5 | 0.32 |
| (1,3495) | 1:23:A:LEU:HD22 | 1:59:A:TYR:HE2 | 5 | 0.32 |
| (1,3495) | 1:23:A:LEU:HD23 | 1:59:A:TYR:HE1 | 5 | 0.32 |
| (1,3495) | 1:23:A:LEU:HD23 | 1:59:A:TYR:HE2 | 5 | 0.32 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 6 | 0.32 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 5 | 0.32 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 14 | 0.32 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 12 | 0.32 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG2 | 16 | 0.32 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG3 | 16 | 0.32 |
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 7 | 0.32 |
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 7 | 0.32 |
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 17 | 0.32 |
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 17 | 0.32 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD11 | 1 | 0.32 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD12 | 1 | 0.32 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD13 | 1 | 0.32 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD11 | 1 | 0.32 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD12 | 1 | 0.32 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD13 | 1 | 0.32 |
| (1,3252) | 1:29:A:TYR:HD1 | 1:68:A:GLY:HA3 | 20 | 0.32 |
| (1,3252) | 1:29:A:TYR:HD2 | 1:68:A:GLY:HA3 | 20 | 0.32 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 1 | 0.32 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 1 | 0.32 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 1 | 0.32 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 1 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 1 | 0.32 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 1 | 0.32 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 1 | 0.32 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 1 | 0.32 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 1 | 0.32 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 8 | 0.32 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 8 | 0.32 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 8 | 0.32 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 19 | 0.32 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 19 | 0.32 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 19 | 0.32 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 19 | 0.32 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 19 | 0.32 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 19 | 0.32 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG21 | 1 | 0.32 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG22 | 1 | 0.32 |
| (1,2658) | 1:9:A:TYR:HD1 | 1:180:A:THR:HG23 | 1 | 0.32 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG21 | 1 | 0.32 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG22 | 1 | 0.32 |
| (1,2658) | 1:9:A:TYR:HD2 | 1:180:A:THR:HG23 | 1 | 0.32 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 6 | 0.32 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 6 | 0.32 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 6 | 0.32 |
| (1,2581) | 1:52:A:GLU:HA | 1:53:A:GLY:HA3 | 14 | 0.32 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 20 | 0.32 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 20 | 0.32 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 20 | 0.32 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 20 | 0.32 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 20 | 0.32 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 20 | 0.32 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 20 | 0.32 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 20 | 0.32 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 20 | 0.32 |
| (1,2539) | 1:20:A:PRO:HG2 | 1:23:A:LEU:HD11 | 7 | 0.32 |
| (1,2539) | 1:20:A:PRO:HG2 | 1:23:A:LEU:HD12 | 7 | 0.32 |
| (1,2539) | 1:20:A:PRO:HG2 | 1:23:A:LEU:HD13 | 7 | 0.32 |
| (1,2539) | 1:20:A:PRO:HG3 | 1:23:A:LEU:HD11 | 7 | 0.32 |
| (1,2539) | 1:20:A:PRO:HG3 | 1:23:A:LEU:HD12 | 7 | 0.32 |
| (1,2539) | 1:20:A:PRO:HG3 | 1:23:A:LEU:HD13 | 7 | 0.32 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 2 | 0.32 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG11 | 2 | 0.32 |
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG12 | 2 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2485) | 1:183:A:GLN:HA | 1:185:A:VAL:HG13 | 2 | 0.32 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 1 | 0.32 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 18 | 0.32 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 19 | 0.32 |
| (1,2289) | 1:42:A:VAL:HG21 | 1:43:A:SER:HA | 3 | 0.32 |
| (1,2289) | 1:42:A:VAL:HG22 | 1:43:A:SER:HA | 3 | 0.32 |
| (1,2289) | 1:42:A:VAL:HG23 | 1:43:A:SER:HA | 3 | 0.32 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 16 | 0.32 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 3 | 0.32 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 15 | 0.32 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 18 | 0.32 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 8 | 0.32 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB2 | 12 | 0.32 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB3 | 12 | 0.32 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 2 | 0.32 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 17 | 0.32 |
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 5 | 0.32 |
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 6 | 0.32 |
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 15 | 0.32 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 18 | 0.32 |
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 8 | 0.32 |
| (1,1831) | 1:7:A:LYS:HB2 | 1:8:A:GLN:H | 17 | 0.32 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 7 | 0.32 |
| (1,1778) | 1:72:A:THR:HB | 1:73:A:GLN:HB3 | 12 | 0.32 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 14 | 0.32 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 14 | 0.32 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 14 | 0.32 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 14 | 0.32 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 14 | 0.32 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 14 | 0.32 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB2 | 16 | 0.32 |
| (1,1777) | 1:184:A:LEU:HD11 | 1:187:A:LYS:HB3 | 16 | 0.32 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB2 | 16 | 0.32 |
| (1,1777) | 1:184:A:LEU:HD12 | 1:187:A:LYS:HB3 | 16 | 0.32 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB2 | 16 | 0.32 |
| (1,1777) | 1:184:A:LEU:HD13 | 1:187:A:LYS:HB3 | 16 | 0.32 |
| (1,1715) | 1:133:A:LEU:H | 1:136:A:GLN:HG2 | 6 | 0.32 |
| (1,1698) | 1:136:A:GLN:HB2 | 1:136:A:GLN:HG2 | 14 | 0.32 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 2 | 0.32 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 5 | 0.32 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 1 | 0.32 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 1 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 1 | 0.32 |
| (1,1604) | 1:61:A:VAL:HA | 1:62:A:GLU:HG2 | 11 | 0.32 |
| (1,1581) | 1:62:A:GLU:HA | 1:62:A:GLU:HG2 | 3 | 0.32 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 5 | 0.32 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 5 | 0.32 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 5 | 0.32 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 14 | 0.32 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 14 | 0.32 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 10 | 0.32 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 12 | 0.32 |
| (1,1526) | 1:63:A:PHE:HB2 | 1:64:A:LEU:H | 16 | 0.32 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 10 | 0.32 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 10 | 0.32 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 10 | 0.32 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 12 | 0.32 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 12 | 0.32 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 12 | 0.32 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 3 | 0.32 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 3 | 0.32 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 3 | 0.32 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB2 | 5 | 0.32 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB3 | 5 | 0.32 |
| (1,1351) | 1:179:A:ASP:HB2 | 1:183:A:GLN:HE21 | 5 | 0.32 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 9 | 0.32 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 13 | 0.32 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 14 | 0.32 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 16 | 0.32 |
| (1,1185) | 1:29:A:TYR:HE1 | 1:68:A:GLY:H | 5 | 0.32 |
| (1,1185) | 1:29:A:TYR:HE2 | 1:68:A:GLY:H | 5 | 0.32 |
| (1,1080) | 1:34:A:TYR:HD1 | 1:38:A:GLU:H | 18 | 0.32 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 8 | 0.32 |
| (1,1040) | 1:52:A:GLU:HB3 | 1:53:A:GLY:H | 17 | 0.32 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 5 | 0.32 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 10 | 0.32 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 15 | 0.32 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 20 | 0.32 |
| (1,815) | 1:91:A:MET:HB2 | 1:93:A:GLU:H | 7 | 0.32 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 3 | 0.32 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 17 | 0.32 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 17 | 0.32 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 17 | 0.32 |
| (1,778) | 1:51:A:PRO:HB3 | 1:54:A:THR:H | 17 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 16 | 0.32 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 16 | 0.32 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 16 | 0.32 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 2 | 0.32 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 5 | 0.32 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 6 | 0.32 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 7 | 0.32 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 11 | 0.32 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 12 | 0.32 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 14 | 0.32 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 16 | 0.32 |
| (1,683) | 1:168:A:SER:H | 1:170:A:MET:HG2 | 5 | 0.32 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 16 | 0.32 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 5 | 0.32 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 18 | 0.32 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 6 | 0.32 |
| (1,606) | 1:137:A:GLN:H | 1:137:A:GLN:HG2 | 7 | 0.32 |
| (1,599) | 1:183:A:GLN:HB3 | 1:184:A:LEU:H | 12 | 0.32 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 8 | 0.32 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 8 | 0.32 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 8 | 0.32 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 11 | 0.32 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 11 | 0.32 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 11 | 0.32 |
| (1,577) | 1:121:A:TYR:HB2 | 1:122:A:ASP:H | 7 | 0.32 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 13 | 0.32 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 13 | 0.32 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 13 | 0.32 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 16 | 0.32 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 16 | 0.32 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 16 | 0.32 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 2 | 0.32 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 2 | 0.32 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 2 | 0.32 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 7 | 0.32 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 7 | 0.32 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 7 | 0.32 |
| (1,441) | 1:34:A:TYR:HE2 | 1:92:A:PHE:H | 16 | 0.32 |
| (1,438) | 1:60:A:HIS:HB2 | 1:75:A:TRP:H | 1 | 0.32 |
| (1,438) | 1:60:A:HIS:HB2 | 1:75:A:TRP:H | 7 | 0.32 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 2 | 0.32 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 2 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 2 | 0.32 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 9 | 0.32 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 9 | 0.32 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 9 | 0.32 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 14 | 0.32 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 14 | 0.32 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 14 | 0.32 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 16 | 0.32 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 16 | 0.32 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 16 | 0.32 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 8 | 0.32 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 8 | 0.32 |
| (1,40) | 1:5:A:ASP:H | 1:7:A:LYS:HB2 | 16 | 0.32 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 16 | 0.31 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 16 | 0.31 |
| (1,3480) | 1:32:A:HIS:HD2 | 1:150:A:PRO:HG3 | 11 | 0.31 |
| (1,3480) | 1:32:A:HIS:HD2 | 1:150:A:PRO:HG3 | 17 | 0.31 |
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 6 | 0.31 |
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 6 | 0.31 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 12 | 0.31 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 12 | 0.31 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 12 | 0.31 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 12 | 0.31 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 12 | 0.31 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 12 | 0.31 |
| (1,3269) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA2 | 16 | 0.31 |
| (1,3269) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA2 | 16 | 0.31 |
| (1,3269) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA2 | 16 | 0.31 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 5 | 0.31 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 5 | 0.31 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 5 | 0.31 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 16 | 0.31 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 16 | 0.31 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 16 | 0.31 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB1 | 13 | 0.31 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB2 | 13 | 0.31 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB3 | 13 | 0.31 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB1 | 13 | 0.31 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB2 | 13 | 0.31 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB3 | 13 | 0.31 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB1 | 13 | 0.31 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB2 | 13 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB3 | 13 | 0.31 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG11 | 3 | 0.31 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG12 | 3 | 0.31 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG13 | 3 | 0.31 |
| (1,2935) | 1:75:A:TRP:HA | 1:78:A:ALA:HA | 18 | 0.31 |
| (1,2908) | 1:175:A:ALA:HA | 1:178:A:ALA:H | 13 | 0.31 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 12 | 0.31 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 12 | 0.31 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 12 | 0.31 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 14 | 0.31 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 14 | 0.31 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 14 | 0.31 |
| (1,2838) | 1:34:A:TYR:HE1 | 1:38:A:GLU:HA | 9 | 0.31 |
| (1,2838) | 1:34:A:TYR:HE2 | 1:38:A:GLU:HA | 9 | 0.31 |
| (1,2827) | 1:72:A:THR:HG21 | 1:134:A:VAL:HG11 | 10 | 0.31 |
| (1,2827) | 1:72:A:THR:HG21 | 1:134:A:VAL:HG12 | 10 | 0.31 |
| (1,2827) | 1:72:A:THR:HG21 | 1:134:A:VAL:HG13 | 10 | 0.31 |
| (1,2827) | 1:72:A:THR:HG22 | 1:134:A:VAL:HG11 | 10 | 0.31 |
| (1,2827) | 1:72:A:THR:HG22 | 1:134:A:VAL:HG12 | 10 | 0.31 |
| (1,2827) | 1:72:A:THR:HG22 | 1:134:A:VAL:HG13 | 10 | 0.31 |
| (1,2827) | 1:72:A:THR:HG23 | 1:134:A:VAL:HG11 | 10 | 0.31 |
| (1,2827) | 1:72:A:THR:HG23 | 1:134:A:VAL:HG12 | 10 | 0.31 |
| (1,2827) | 1:72:A:THR:HG23 | 1:134:A:VAL:HG13 | 10 | 0.31 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 9 | 0.31 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 15 | 0.31 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 6 | 0.31 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 6 | 0.31 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 6 | 0.31 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 6 | 0.31 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 6 | 0.31 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 6 | 0.31 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 6 | 0.31 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 6 | 0.31 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 6 | 0.31 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 13 | 0.31 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 13 | 0.31 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 13 | 0.31 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 12 | 0.31 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 12 | 0.31 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 12 | 0.31 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 12 | 0.31 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 12 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 12 | 0.31 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 4 | 0.31 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 4 | 0.31 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 4 | 0.31 |
| (1,2621) | 1:101:A:VAL:HG21 | 1:106:A:ASP:H | 12 | 0.31 |
| (1,2621) | 1:101:A:VAL:HG22 | 1:106:A:ASP:H | 12 | 0.31 |
| (1,2621) | 1:101:A:VAL:HG23 | 1:106:A:ASP:H | 12 | 0.31 |
| (1,2581) | 1:52:A:GLU:HA | 1:53:A:GLY:HA3 | 9 | 0.31 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 8 | 0.31 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 15 | 0.31 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 16 | 0.31 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 5 | 0.31 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 5 | 0.31 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 5 | 0.31 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 11 | 0.31 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 11 | 0.31 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 11 | 0.31 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 12 | 0.31 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 12 | 0.31 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 12 | 0.31 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 20 | 0.31 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 20 | 0.31 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 20 | 0.31 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 18 | 0.31 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 18 | 0.31 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 18 | 0.31 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 18 | 0.31 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 18 | 0.31 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 18 | 0.31 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 2 | 0.31 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 2 | 0.31 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 2 | 0.31 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 16 | 0.31 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 16 | 0.31 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 16 | 0.31 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 20 | 0.31 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 20 | 0.31 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 20 | 0.31 |
| (1,2452) | 1:149:A:VAL:HG11 | 1:150:A:PRO:HG3 | 14 | 0.31 |
| (1,2452) | 1:149:A:VAL:HG12 | 1:150:A:PRO:HG3 | 14 | 0.31 |
| (1,2452) | 1:149:A:VAL:HG13 | 1:150:A:PRO:HG3 | 14 | 0.31 |
| (1,2452) | 1:149:A:VAL:HG21 | 1:150:A:PRO:HG3 | 14 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2452) | 1:149:A:VAL:HG22 | 1:150:A:PRO:HG3 | 14 | 0.31 |
| (1,2452) | 1:149:A:VAL:HG23 | 1:150:A:PRO:HG3 | 14 | 0.31 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 8 | 0.31 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 19 | 0.31 |
| (1,2392) | 1:31:A:PRO:HA | 1:34:A:TYR:HA | 9 | 0.31 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 13 | 0.31 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 20 | 0.31 |
| (1,2369) | 1:157:A:LYS:HG2 | 1:158:A:TYR:HA | 9 | 0.31 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 17 | 0.31 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 15 | 0.31 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 15 | 0.31 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 15 | 0.31 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 15 | 0.31 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 15 | 0.31 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 15 | 0.31 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 20 | 0.31 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 15 | 0.31 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 9 | 0.31 |
| (1,2168) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HG2 | 12 | 0.31 |
| (1,2168) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HG2 | 12 | 0.31 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 17 | 0.31 |
| (1,2072) | 1:93:A:GLU:HA | 1:97:A:LYS:HD2 | 1 | 0.31 |
| (1,2072) | 1:93:A:GLU:HA | 1:97:A:LYS:HD2 | 16 | 0.31 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 7 | 0.31 |
| (1,2047) | 1:119:A:GLU:HB3 | 1:120:A:ASP:HA | 14 | 0.31 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 20 | 0.31 |
| (1,2015) | 1:117:A:LYS:HB2 | 1:117:A:LYS:HD3 | 15 | 0.31 |
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 2 | 0.31 |
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 20 | 0.31 |
| (1,1930) | 1:186:A:GLU:HB3 | 1:187:A:LYS:H | 9 | 0.31 |
| (1,1869) | 1:73:A:GLN:HG2 | 1:134:A:VAL:HG21 | 19 | 0.31 |
| (1,1869) | 1:73:A:GLN:HG2 | 1:134:A:VAL:HG22 | 19 | 0.31 |
| (1,1869) | 1:73:A:GLN:HG2 | 1:134:A:VAL:HG23 | 19 | 0.31 |
| (1,1867) | 1:37:A:GLU:HB2 | 1:38:A:GLU:HA | 2 | 0.31 |
| (1,1843) | 1:60:A:HIS:HB2 | 1:72:A:THR:HA | 3 | 0.31 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 5 | 0.31 |
| (1,1778) | 1:72:A:THR:HB | 1:73:A:GLN:HB3 | 6 | 0.31 |
| (1,1751) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HG2 | 18 | 0.31 |
| (1,1751) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HG3 | 18 | 0.31 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 6 | 0.31 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 10 | 0.31 |
| (1,1695) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HE22 | 12 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1695) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HE22 | 19 | 0.31 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG2 | 1 | 0.31 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG3 | 1 | 0.31 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG2 | 2 | 0.31 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG3 | 2 | 0.31 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG2 | 15 | 0.31 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG3 | 15 | 0.31 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 12 | 0.31 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 10 | 0.31 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 12 | 0.31 |
| (1,1513) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB2 | 2 | 0.31 |
| (1,1513) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB2 | 2 | 0.31 |
| (1,1513) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB2 | 2 | 0.31 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 17 | 0.31 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 8 | 0.31 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 8 | 0.31 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 8 | 0.31 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 19 | 0.31 |
| (1,1450) | 1:42:A:VAL:HA | 1:45:A:ASN:HB3 | 10 | 0.31 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 6 | 0.31 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 6 | 0.31 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 6 | 0.31 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 6 | 0.31 |
| (1,1334) | 1:67:A:LEU:HB3 | 1:70:A:ASP:HB3 | 3 | 0.31 |
| (1,1265) | 1:64:A:LEU:HB3 | 1:65:A:GLY:HA2 | 10 | 0.31 |
| (1,1258) | 1:163:A:GLN:HG2 | 1:164:A:GLY:HA3 | 19 | 0.31 |
| (1,1258) | 1:163:A:GLN:HG3 | 1:164:A:GLY:HA3 | 19 | 0.31 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 9 | 0.31 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 8 | 0.31 |
| (1,1141) | 1:126:A:ASN:H | 1:127:A:SER:HB3 | 18 | 0.31 |
| (1,1080) | 1:34:A:TYR:HD1 | 1:38:A:GLU:H | 19 | 0.31 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 5 | 0.31 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 9 | 0.31 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 19 | 0.31 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 13 | 0.31 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG21 | 8 | 0.31 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG22 | 8 | 0.31 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG23 | 8 | 0.31 |
| (1,938) | 1:112:A:VAL:HG11 | 1:118:A:GLY:H | 1 | 0.31 |
| (1,938) | 1:112:A:VAL:HG12 | 1:118:A:GLY:H | 1 | 0.31 |
| (1,938) | 1:112:A:VAL:HG13 | 1:118:A:GLY:H | 1 | 0.31 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 19 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 19 | 0.31 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 19 | 0.31 |
| (1,815) | 1:91:A:MET:HB2 | 1:93:A:GLU:H | 19 | 0.31 |
| (1,799) | 1:49:A:LYS:HG2 | 1:179:A:ASP:H | 17 | 0.31 |
| (1,799) | 1:49:A:LYS:HG3 | 1:179:A:ASP:H | 17 | 0.31 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 8 | 0.31 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 9 | 0.31 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 13 | 0.31 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 17 | 0.31 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 19 | 0.31 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 7 | 0.31 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 10 | 0.31 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 11 | 0.31 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 14 | 0.31 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 17 | 0.31 |
| (1,599) | 1:183:A:GLN:HB3 | 1:184:A:LEU:H | 9 | 0.31 |
| (1,553) | 1:42:A:VAL:HG21 | 1:46:A:VAL:H | 7 | 0.31 |
| (1,553) | 1:42:A:VAL:HG22 | 1:46:A:VAL:H | 7 | 0.31 |
| (1,553) | 1:42:A:VAL:HG23 | 1:46:A:VAL:H | 7 | 0.31 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 1 | 0.31 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 1 | 0.31 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 1 | 0.31 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 3 | 0.31 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 3 | 0.31 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 3 | 0.31 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 5 | 0.31 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 5 | 0.31 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 5 | 0.31 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 11 | 0.31 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 11 | 0.31 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 11 | 0.31 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 18 | 0.31 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 18 | 0.31 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 18 | 0.31 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 11 | 0.31 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 11 | 0.31 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 11 | 0.31 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 12 | 0.31 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 12 | 0.31 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 12 | 0.31 |
| (1,353) | 1:108:A:ARG:HG3 | 1:112:A:VAL:H | 18 | 0.31 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 2 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 2 | 0.31 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 2 | 0.31 |
| (1,285) | 1:152:A:MET:H | 1:152:A:MET:HB3 | 17 | 0.31 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 10 | 0.31 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 12 | 0.31 |
| (1,216) | 1:34:A:TYR:H | 1:96:A:GLN:HE21 | 4 | 0.31 |
| (1,164) | 1:69:A:LYS:H | 1:69:A:LYS:HB3 | 1 | 0.31 |
| (1,78) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 7 | 0.31 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 20 | 0.31 |
| (1,3530) | 1:73:A:GLN:HE22 | 1:125:A:TRP:HZ2 | 18 | 0.3 |
| (1,3523) | 1:73:A:GLN:HE21 | 1:125:A:TRP:HZ2 | 11 | 0.3 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 19 | 0.3 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 19 | 0.3 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 19 | 0.3 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 19 | 0.3 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 19 | 0.3 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 19 | 0.3 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 6 | 0.3 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 6 | 0.3 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 13 | 0.3 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG2 | 20 | 0.3 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG3 | 20 | 0.3 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 2 | 0.3 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 2 | 0.3 |
| (1,3229) | 1:88:A:THR:H | 1:90:A:PRO:HD3 | 10 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 4 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 4 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 4 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 4 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 4 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 4 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 4 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 4 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 4 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 13 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 13 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 13 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 13 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 13 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 13 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 13 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 13 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 13 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 17 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 17 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 17 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 17 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 17 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 17 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 17 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 17 | 0.3 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 17 | 0.3 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 19 | 0.3 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 19 | 0.3 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 19 | 0.3 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 19 | 0.3 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 19 | 0.3 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 19 | 0.3 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 19 | 0.3 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 19 | 0.3 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 19 | 0.3 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 5 | 0.3 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 5 | 0.3 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 5 | 0.3 |
| (1,2838) | 1:34:A:TYR:HE1 | 1:38:A:GLU:HA | 5 | 0.3 |
| (1,2838) | 1:34:A:TYR:HE2 | 1:38:A:GLU:HA | 5 | 0.3 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 14 | 0.3 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 14 | 0.3 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 14 | 0.3 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG21 | 18 | 0.3 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG22 | 18 | 0.3 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG23 | 18 | 0.3 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG21 | 18 | 0.3 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG22 | 18 | 0.3 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG23 | 18 | 0.3 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG21 | 18 | 0.3 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG22 | 18 | 0.3 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG23 | 18 | 0.3 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 16 | 0.3 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 16 | 0.3 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 16 | 0.3 |
| (1,2632) | 1:101:A:VAL:HG21 | 1:107:A:ILE:H | 12 | 0.3 |
| (1,2632) | 1:101:A:VAL:HG22 | 1:107:A:ILE:H | 12 | 0.3 |
| (1,2632) | 1:101:A:VAL:HG23 | 1:107:A:ILE:H | 12 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2622) | 1:149:A:VAL:HA | 1:151:A:ALA:H | 4 | 0.3 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 1 | 0.3 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 2 | 0.3 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 4 | 0.3 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 5 | 0.3 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 9 | 0.3 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 10 | 0.3 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 12 | 0.3 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 14 | 0.3 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 17 | 0.3 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 19 | 0.3 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 2 | 0.3 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 2 | 0.3 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 2 | 0.3 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 7 | 0.3 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 7 | 0.3 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 7 | 0.3 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 7 | 0.3 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 7 | 0.3 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 7 | 0.3 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 7 | 0.3 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 7 | 0.3 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 7 | 0.3 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD21 | 4 | 0.3 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD22 | 4 | 0.3 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD23 | 4 | 0.3 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD21 | 6 | 0.3 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD22 | 6 | 0.3 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD23 | 6 | 0.3 |
| (1,2479) | 1:8:A:GLN:HA | 1:8:A:GLN:HG2 | 13 | 0.3 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 17 | 0.3 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 9 | 0.3 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 5 | 0.3 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 5 | 0.3 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 5 | 0.3 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 17 | 0.3 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 17 | 0.3 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 17 | 0.3 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 17 | 0.3 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 17 | 0.3 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 17 | 0.3 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 5 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2171) | 1:86:A:LYS:H | 1:87:A:ILE:HG12 | 14 | 0.3 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 12 | 0.3 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG21 | 18 | 0.3 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG22 | 18 | 0.3 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG23 | 18 | 0.3 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG21 | 18 | 0.3 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG22 | 18 | 0.3 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG23 | 18 | 0.3 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 1 | 0.3 |
| (1,2020) | 1:86:A:LYS:H | 1:86:A:LYS:HD2 | 12 | 0.3 |
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 13 | 0.3 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 12 | 0.3 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 12 | 0.3 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 12 | 0.3 |
| (1,1832) | 1:124:A:ALA:HB1 | 1:130:A:VAL:HB | 3 | 0.3 |
| (1,1832) | 1:124:A:ALA:HB2 | 1:130:A:VAL:HB | 3 | 0.3 |
| (1,1832) | 1:124:A:ALA:HB3 | 1:130:A:VAL:HB | 3 | 0.3 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 11 | 0.3 |
| (1,1744) | 1:134:A:VAL:HA | 1:137:A:GLN:HG2 | 14 | 0.3 |
| (1,1698) | 1:136:A:GLN:HB2 | 1:136:A:GLN:HG2 | 4 | 0.3 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 8 | 0.3 |
| (1,1690) | 1:45:A:ASN:HA | 1:48:A:GLN:HG2 | 13 | 0.3 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG2 | 11 | 0.3 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG3 | 11 | 0.3 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG2 | 12 | 0.3 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG3 | 12 | 0.3 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG2 | 13 | 0.3 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG3 | 13 | 0.3 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG2 | 16 | 0.3 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG3 | 16 | 0.3 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG2 | 19 | 0.3 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG3 | 19 | 0.3 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG2 | 20 | 0.3 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG3 | 20 | 0.3 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 2 | 0.3 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 14 | 0.3 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 9 | 0.3 |
| (1,1632) | 1:31:A:PRO:HA | 1:96:A:GLN:HG2 | 10 | 0.3 |
| (1,1563) | 1:152:A:MET:HB3 | 1:160:A:LEU:HB3 | 18 | 0.3 |
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 2 | 0.3 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 2 | 0.3 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 2 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1513) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB2 | 12 | 0.3 |
| (1,1513) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB2 | 12 | 0.3 |
| (1,1513) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB2 | 12 | 0.3 |
| (1,1513) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB2 | 16 | 0.3 |
| (1,1513) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB2 | 16 | 0.3 |
| (1,1513) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB2 | 16 | 0.3 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 1 | 0.3 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 1 | 0.3 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 1 | 0.3 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 3 | 0.3 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 3 | 0.3 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 3 | 0.3 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG21 | 11 | 0.3 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG22 | 11 | 0.3 |
| (1,1443) | 1:45:A:ASN:HB2 | 1:174:A:VAL:HG23 | 11 | 0.3 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE2 | 12 | 0.3 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE3 | 12 | 0.3 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE2 | 12 | 0.3 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE3 | 12 | 0.3 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE2 | 12 | 0.3 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE3 | 12 | 0.3 |
| (1,1337) | 1:67:A:LEU:HB3 | 1:70:A:ASP:HB2 | 18 | 0.3 |
| (1,1331) | 1:70:A:ASP:HB3 | 1:72:A:THR:H | 19 | 0.3 |
| (1,1258) | 1:163:A:GLN:HG2 | 1:164:A:GLY:HA3 | 10 | 0.3 |
| (1,1258) | 1:163:A:GLN:HG3 | 1:164:A:GLY:HA3 | 10 | 0.3 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 12 | 0.3 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 15 | 0.3 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 18 | 0.3 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG11 | 10 | 0.3 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG12 | 10 | 0.3 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG13 | 10 | 0.3 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 14 | 0.3 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 17 | 0.3 |
| (1,1005) | 1:46:A:VAL:HG21 | 1:48:A:GLN:H | 15 | 0.3 |
| (1,1005) | 1:46:A:VAL:HG22 | 1:48:A:GLN:H | 15 | 0.3 |
| (1,1005) | 1:46:A:VAL:HG23 | 1:48:A:GLN:H | 15 | 0.3 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 18 | 0.3 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 12 | 0.3 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 12 | 0.3 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 12 | 0.3 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 17 | 0.3 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 17 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 17 | 0.3 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 19 | 0.3 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 10 | 0.3 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 14 | 0.3 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 7 | 0.3 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 7 | 0.3 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 7 | 0.3 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 16 | 0.3 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 16 | 0.3 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 16 | 0.3 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD21 | 8 | 0.3 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD22 | 8 | 0.3 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD23 | 8 | 0.3 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 8 | 0.3 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 20 | 0.3 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 1 | 0.3 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG21 | 19 | 0.3 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG22 | 19 | 0.3 |
| (1,512) | 1:26:A:PHE:H | 1:149:A:VAL:HG23 | 19 | 0.3 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 4 | 0.3 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 4 | 0.3 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 4 | 0.3 |
| (1,485) | 1:4:A:THR:H | 1:7:A:LYS:HB2 | 20 | 0.3 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG11 | 8 | 0.3 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG12 | 8 | 0.3 |
| (1,468) | 1:42:A:VAL:H | 1:42:A:VAL:HG13 | 8 | 0.3 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 9 | 0.3 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 9 | 0.3 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 9 | 0.3 |
| (1,259) | 1:69:A:LYS:HD2 | 1:70:A:ASP:H | 16 | 0.3 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 16 | 0.3 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 5 | 0.3 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 20 | 0.3 |
| (1,216) | 1:34:A:TYR:H | 1:96:A:GLN:HE21 | 8 | 0.3 |
| (1,188) | 1:60:A:HIS:H | 1:137:A:GLN:HG3 | 5 | 0.3 |
| (1,164) | 1:69:A:LYS:H | 1:69:A:LYS:HB3 | 14 | 0.3 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 19 | 0.3 |
| (1,118) | 1:159:A:GLN:H | 1:184:A:LEU:HD21 | 5 | 0.3 |
| (1,118) | 1:159:A:GLN:H | 1:184:A:LEU:HD22 | 5 | 0.3 |
| (1,118) | 1:159:A:GLN:H | 1:184:A:LEU:HD23 | 5 | 0.3 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG11 | 6 | 0.3 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG12 | 6 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG13 | 6 | 0.3 |
| (1,78) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 17 | 0.3 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 1 | 0.3 |
| (1,3530) | 1:73:A:GLN:HE22 | 1:125:A:TRP:HZ2 | 16 | 0.29 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 1 | 0.29 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 1 | 0.29 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 1 | 0.29 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 1 | 0.29 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 1 | 0.29 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 1 | 0.29 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD11 | 15 | 0.29 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD12 | 15 | 0.29 |
| (1,3498) | 1:158:A:TYR:HE1 | 1:184:A:LEU:HD13 | 15 | 0.29 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD11 | 15 | 0.29 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD12 | 15 | 0.29 |
| (1,3498) | 1:158:A:TYR:HE2 | 1:184:A:LEU:HD13 | 15 | 0.29 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 10 | 0.29 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 10 | 0.29 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 10 | 0.29 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD11 | 13 | 0.29 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD12 | 13 | 0.29 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD13 | 13 | 0.29 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD11 | 13 | 0.29 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD12 | 13 | 0.29 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD13 | 13 | 0.29 |
| (1,3297) | 1:23:A:LEU:HB2 | 1:153:A:TYR:H | 3 | 0.29 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 16 | 0.29 |
| (1,3277) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA3 | 5 | 0.29 |
| (1,3277) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA3 | 5 | 0.29 |
| (1,3277) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA3 | 5 | 0.29 |
| (1,3150) | 1:59:A:TYR:HA | 1:137:A:GLN:HG3 | 6 | 0.29 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 3 | 0.29 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 3 | 0.29 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 3 | 0.29 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 3 | 0.29 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 3 | 0.29 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 3 | 0.29 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE1 | 3 | 0.29 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE2 | 3 | 0.29 |
| (1,3073) | 1:43:A:SER:HB2 | 1:56:A:MET:HE3 | 3 | 0.29 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE1 | 3 | 0.29 |
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE2 | 3 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3073) | 1:43:A:SER:HB3 | 1:56:A:MET:HE3 | 3 | 0.29 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 3 | 0.29 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 3 | 0.29 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 3 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG21 | 14 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG22 | 14 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG23 | 14 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG21 | 14 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG22 | 14 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG23 | 14 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG21 | 14 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG22 | 14 | 0.29 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG23 | 14 | 0.29 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 11 | 0.29 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 11 | 0.29 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 11 | 0.29 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 11 | 0.29 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 11 | 0.29 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 11 | 0.29 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 11 | 0.29 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 11 | 0.29 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 11 | 0.29 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 11 | 0.29 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 11 | 0.29 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 11 | 0.29 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 11 | 0.29 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 11 | 0.29 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 11 | 0.29 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 11 | 0.29 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 11 | 0.29 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 11 | 0.29 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG11 | 10 | 0.29 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG12 | 10 | 0.29 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG13 | 10 | 0.29 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 10 | 0.29 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 10 | 0.29 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 10 | 0.29 |
| (1,2908) | 1:175:A:ALA:HA | 1:178:A:ALA:H | 11 | 0.29 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 20 | 0.29 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 3 | 0.29 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 3 | 0.29 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 3 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 15 | 0.29 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 15 | 0.29 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 15 | 0.29 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 9 | 0.29 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 9 | 0.29 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 9 | 0.29 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 8 | 0.29 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 8 | 0.29 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 8 | 0.29 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 8 | 0.29 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 8 | 0.29 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 8 | 0.29 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 3 | 0.29 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 3 | 0.29 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 3 | 0.29 |
| (1,2621) | 1:101:A:VAL:HG21 | 1:106:A:ASP:H | 9 | 0.29 |
| (1,2621) | 1:101:A:VAL:HG22 | 1:106:A:ASP:H | 9 | 0.29 |
| (1,2621) | 1:101:A:VAL:HG23 | 1:106:A:ASP:H | 9 | 0.29 |
| (1,2621) | 1:101:A:VAL:HG21 | 1:106:A:ASP:H | 10 | 0.29 |
| (1,2621) | 1:101:A:VAL:HG22 | 1:106:A:ASP:H | 10 | 0.29 |
| (1,2621) | 1:101:A:VAL:HG23 | 1:106:A:ASP:H | 10 | 0.29 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 14 | 0.29 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 14 | 0.29 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 14 | 0.29 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 3 | 0.29 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 6 | 0.29 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 11 | 0.29 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 20 | 0.29 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 6 | 0.29 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 6 | 0.29 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 6 | 0.29 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 9 | 0.29 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 20 | 0.29 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 7 | 0.29 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 7 | 0.29 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 7 | 0.29 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 9 | 0.29 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 9 | 0.29 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 9 | 0.29 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 9 | 0.29 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 9 | 0.29 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 9 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 3 | 0.29 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 11 | 0.29 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 12 | 0.29 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 20 | 0.29 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 5 | 0.29 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 9 | 0.29 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 3 | 0.29 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 7 | 0.29 |
| (1,1988) | 1:136:A:GLN:H | 1:136:A:GLN:HB2 | 17 | 0.29 |
| (1,1981) | 1:187:A:LYS:H | 1:187:A:LYS:HD3 | 9 | 0.29 |
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 18 | 0.29 |
| (1,1791) | 1:56:A:MET:HA | 1:56:A:MET:HG3 | 16 | 0.29 |
| (1,1699) | 1:135:A:ALA:HB1 | 1:136:A:GLN:HG2 | 16 | 0.29 |
| (1,1699) | 1:135:A:ALA:HB2 | 1:136:A:GLN:HG2 | 16 | 0.29 |
| (1,1699) | 1:135:A:ALA:HB3 | 1:136:A:GLN:HG2 | 16 | 0.29 |
| (1,1698) | 1:136:A:GLN:HB2 | 1:136:A:GLN:HG2 | 12 | 0.29 |
| (1,1695) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HE22 | 10 | 0.29 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG2 | 10 | 0.29 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG3 | 10 | 0.29 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG2 | 14 | 0.29 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG3 | 14 | 0.29 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 17 | 0.29 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 4 | 0.29 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 5 | 0.29 |
| (1,1576) | 1:119:A:GLU:HG2 | 1:120:A:ASP:H | 8 | 0.29 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 20 | 0.29 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 20 | 0.29 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 20 | 0.29 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 5 | 0.29 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 18 | 0.29 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 2 | 0.29 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 17 | 0.29 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 17 | 0.29 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 17 | 0.29 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 2 | 0.29 |
| (1,1427) | 1:143:A:ASP:HB2 | 1:145:A:GLN:HE22 | 9 | 0.29 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 9 | 0.29 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 9 | 0.29 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 9 | 0.29 |
| (1,1366) | 1:34:A:TYR:HE1 | 1:97:A:LYS:HE3 | 3 | 0.29 |
| (1,1366) | 1:34:A:TYR:HE2 | 1:97:A:LYS:HE3 | 3 | 0.29 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG11 | 7 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG12 | 7 | 0.29 |
| (1,1247) | 1:115:A:GLY:H | 1:116:A:VAL:HG13 | 7 | 0.29 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 13 | 0.29 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 2 | 0.29 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 19 | 0.29 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG11 | 17 | 0.29 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG12 | 17 | 0.29 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG13 | 17 | 0.29 |
| (1,1164) | 1:27:A:SER:H | 1:30:A:CYS:HB3 | 19 | 0.29 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 4 | 0.29 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 11 | 0.29 |
| (1,1040) | 1:52:A:GLU:HB3 | 1:53:A:GLY:H | 1 | 0.29 |
| (1,1005) | 1:46:A:VAL:HG21 | 1:48:A:GLN:H | 3 | 0.29 |
| (1,1005) | 1:46:A:VAL:HG22 | 1:48:A:GLN:H | 3 | 0.29 |
| (1,1005) | 1:46:A:VAL:HG23 | 1:48:A:GLN:H | 3 | 0.29 |
| (1,1005) | 1:46:A:VAL:HG21 | 1:48:A:GLN:H | 14 | 0.29 |
| (1,1005) | 1:46:A:VAL:HG22 | 1:48:A:GLN:H | 14 | 0.29 |
| (1,1005) | 1:46:A:VAL:HG23 | 1:48:A:GLN:H | 14 | 0.29 |
| (1,1005) | 1:46:A:VAL:HG21 | 1:48:A:GLN:H | 17 | 0.29 |
| (1,1005) | 1:46:A:VAL:HG22 | 1:48:A:GLN:H | 17 | 0.29 |
| (1,1005) | 1:46:A:VAL:HG23 | 1:48:A:GLN:H | 17 | 0.29 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 18 | 0.29 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 4 | 0.29 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 4 | 0.29 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 4 | 0.29 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 9 | 0.29 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 9 | 0.29 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 9 | 0.29 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 6 | 0.29 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 7 | 0.29 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 7 | 0.29 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 7 | 0.29 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 16 | 0.29 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 18 | 0.29 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 10 | 0.29 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 8 | 0.29 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 7 | 0.29 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 7 | 0.29 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 7 | 0.29 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 18 | 0.29 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 18 | 0.29 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 18 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,555) | 1:174:A:VAL:HG21 | 1:178:A:ALA:H | 7 | 0.29 |
| (1,555) | 1:174:A:VAL:HG22 | 1:178:A:ALA:H | 7 | 0.29 |
| (1,555) | 1:174:A:VAL:HG23 | 1:178:A:ALA:H | 7 | 0.29 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 11 | 0.29 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 11 | 0.29 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 11 | 0.29 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 17 | 0.29 |
| (1,401) | 1:117:A:LYS:HB2 | 1:120:A:ASP:H | 5 | 0.29 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG11 | 15 | 0.29 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG12 | 15 | 0.29 |
| (1,371) | 1:101:A:VAL:H | 1:101:A:VAL:HG13 | 15 | 0.29 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 13 | 0.29 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 13 | 0.29 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 13 | 0.29 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 15 | 0.29 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 4 | 0.29 |
| (1,216) | 1:34:A:TYR:H | 1:96:A:GLN:HE21 | 5 | 0.29 |
| (1,161) | 1:29:A:TYR:HE1 | 1:69:A:LYS:H | 6 | 0.29 |
| (1,161) | 1:29:A:TYR:HE2 | 1:69:A:LYS:H | 6 | 0.29 |
| (1,83) | 1:6:A:GLY:H | 1:11:A:THR:H | 1 | 0.29 |
| (1,78) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 2 | 0.29 |
| (1,78) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 8 | 0.29 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 2 | 0.29 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 11 | 0.29 |
| (1,35) | 1:117:A:LYS:H | 1:117:A:LYS:HB3 | 5 | 0.29 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 8 | 0.28 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 8 | 0.28 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 8 | 0.28 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 8 | 0.28 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 8 | 0.28 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 8 | 0.28 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 5 | 0.28 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 5 | 0.28 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 12 | 0.28 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 12 | 0.28 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 3 | 0.28 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 3 | 0.28 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 2 | 0.28 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 15 | 0.28 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 15 | 0.28 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 15 | 0.28 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 15 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 15 | 0.28 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 15 | 0.28 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 10 | 0.28 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 10 | 0.28 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 10 | 0.28 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG21 | 11 | 0.28 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG22 | 11 | 0.28 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG23 | 11 | 0.28 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG21 | 11 | 0.28 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG22 | 11 | 0.28 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG23 | 11 | 0.28 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG21 | 11 | 0.28 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG22 | 11 | 0.28 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG23 | 11 | 0.28 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 20 | 0.28 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 20 | 0.28 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 20 | 0.28 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 20 | 0.28 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 20 | 0.28 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 20 | 0.28 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 20 | 0.28 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 20 | 0.28 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 20 | 0.28 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 12 | 0.28 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 7 | 0.28 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG11 | 3 | 0.28 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG12 | 3 | 0.28 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG13 | 3 | 0.28 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 14 | 0.28 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 14 | 0.28 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 14 | 0.28 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 14 | 0.28 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 14 | 0.28 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 14 | 0.28 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 15 | 0.28 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 15 | 0.28 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 15 | 0.28 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 15 | 0.28 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 15 | 0.28 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 15 | 0.28 |
| (1,2699) | 1:134:A:VAL:HG11 | 1:138:A:GLU:HG3 | 16 | 0.28 |
| (1,2699) | 1:134:A:VAL:HG12 | 1:138:A:GLU:HG3 | 16 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2699) | 1:134:A:VAL:HG13 | 1:138:A:GLU:HG3 | 16 | 0.28 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 14 | 0.28 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 14 | 0.28 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 14 | 0.28 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG21 | 20 | 0.28 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG22 | 20 | 0.28 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG23 | 20 | 0.28 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG21 | 20 | 0.28 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG22 | 20 | 0.28 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG23 | 20 | 0.28 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG21 | 20 | 0.28 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG22 | 20 | 0.28 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG23 | 20 | 0.28 |
| (1,2632) | 1:101:A:VAL:HG21 | 1:107:A:ILE:H | 5 | 0.28 |
| (1,2632) | 1:101:A:VAL:HG22 | 1:107:A:ILE:H | 5 | 0.28 |
| (1,2632) | 1:101:A:VAL:HG23 | 1:107:A:ILE:H | 5 | 0.28 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 2 | 0.28 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 2 | 0.28 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 2 | 0.28 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 5 | 0.28 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 5 | 0.28 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 5 | 0.28 |
| (1,2606) | 1:187:A:LYS:HA | 1:187:A:LYS:HG3 | 8 | 0.28 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 1 | 0.28 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 1 | 0.28 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 1 | 0.28 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 1 | 0.28 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 1 | 0.28 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 1 | 0.28 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 1 | 0.28 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 1 | 0.28 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 1 | 0.28 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 4 | 0.28 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 4 | 0.28 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 4 | 0.28 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 4 | 0.28 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 4 | 0.28 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 4 | 0.28 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 4 | 0.28 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 4 | 0.28 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 4 | 0.28 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 18 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 18 | 0.28 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 18 | 0.28 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 18 | 0.28 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 18 | 0.28 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 18 | 0.28 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 18 | 0.28 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 18 | 0.28 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 18 | 0.28 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 13 | 0.28 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 1 | 0.28 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 1 | 0.28 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 1 | 0.28 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 14 | 0.28 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 14 | 0.28 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 14 | 0.28 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 13 | 0.28 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 13 | 0.28 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 13 | 0.28 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 13 | 0.28 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 13 | 0.28 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 13 | 0.28 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 13 | 0.28 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 13 | 0.28 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 13 | 0.28 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 7 | 0.28 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 11 | 0.28 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 3 | 0.28 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 11 | 0.28 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 14 | 0.28 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 8 | 0.28 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 13 | 0.28 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD11 | 18 | 0.28 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD12 | 18 | 0.28 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD13 | 18 | 0.28 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD21 | 18 | 0.28 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD22 | 18 | 0.28 |
| (1,2150) | 1:79:A:ILE:HG12 | 1:133:A:LEU:HD23 | 18 | 0.28 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 18 | 0.28 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG21 | 2 | 0.28 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG22 | 2 | 0.28 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG23 | 2 | 0.28 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG21 | 2 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG22 | 2 | 0.28 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG23 | 2 | 0.28 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 9 | 0.28 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 13 | 0.28 |
| (1,2020) | 1:86:A:LYS:H | 1:86:A:LYS:HD2 | 11 | 0.28 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 4 | 0.28 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 7 | 0.28 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 2 | 0.28 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 2 | 0.28 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 2 | 0.28 |
| (1,1873) | 1:46:A:VAL:HA | 1:49:A:LYS:HB3 | 15 | 0.28 |
| (1,1867) | 1:37:A:GLU:HB2 | 1:38:A:GLU:HA | 20 | 0.28 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 10 | 0.28 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 14 | 0.28 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 19 | 0.28 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE1 | 20 | 0.28 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE2 | 20 | 0.28 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE3 | 20 | 0.28 |
| (1,1744) | 1:134:A:VAL:HA | 1:137:A:GLN:HG2 | 2 | 0.28 |
| (1,1698) | 1:136:A:GLN:HB2 | 1:136:A:GLN:HG2 | 5 | 0.28 |
| (1,1698) | 1:136:A:GLN:HB2 | 1:136:A:GLN:HG2 | 20 | 0.28 |
| (1,1695) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HE22 | 2 | 0.28 |
| (1,1695) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HE22 | 5 | 0.28 |
| (1,1695) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HE22 | 18 | 0.28 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 7 | 0.28 |
| (1,1565) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 11 | 0.28 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 18 | 0.28 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 18 | 0.28 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 18 | 0.28 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 11 | 0.28 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 11 | 0.28 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 9 | 0.28 |
| (1,1485) | 1:28:A:PHE:HB2 | 1:95:A:VAL:HB | 9 | 0.28 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 6 | 0.28 |
| (1,1474) | 1:161:A:ASN:HB2 | 1:161:A:ASN:HD22 | 11 | 0.28 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 18 | 0.28 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 18 | 0.28 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 18 | 0.28 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 17 | 0.28 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 17 | 0.28 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 17 | 0.28 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 12 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 6 | 0.28 |
| (1,1213) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE21 | 5 | 0.28 |
| (1,1213) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE21 | 5 | 0.28 |
| (1,1213) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE21 | 5 | 0.28 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 4 | 0.28 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 5 | 0.28 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 7 | 0.28 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 20 | 0.28 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 2 | 0.28 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 3 | 0.28 |
| (1,1058) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HA | 4 | 0.28 |
| (1,1040) | 1:52:A:GLU:HB3 | 1:53:A:GLY:H | 2 | 0.28 |
| (1,991) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HD22 | 3 | 0.28 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 4 | 0.28 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 4 | 0.28 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 4 | 0.28 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 10 | 0.28 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 10 | 0.28 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 10 | 0.28 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 14 | 0.28 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 14 | 0.28 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 14 | 0.28 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 12 | 0.28 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 12 | 0.28 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 12 | 0.28 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG11 | 7 | 0.28 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG12 | 7 | 0.28 |
| (1,705) | 1:45:A:ASN:H | 1:46:A:VAL:HG13 | 7 | 0.28 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 7 | 0.28 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 20 | 0.28 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 3 | 0.28 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 12 | 0.28 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 19 | 0.28 |
| (1,599) | 1:183:A:GLN:HB3 | 1:184:A:LEU:H | 3 | 0.28 |
| (1,599) | 1:183:A:GLN:HB3 | 1:184:A:LEU:H | 19 | 0.28 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 10 | 0.28 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 10 | 0.28 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 10 | 0.28 |
| (1,492) | 1:138:A:GLU:HB2 | 1:140:A:ALA:H | 2 | 0.28 |
| (1,485) | 1:4:A:THR:H | 1:7:A:LYS:HB2 | 13 | 0.28 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 17 | 0.28 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 19 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 16 | 0.28 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 16 | 0.28 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 16 | 0.28 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 17 | 0.28 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 17 | 0.28 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 17 | 0.28 |
| (1,285) | 1:152:A:MET:H | 1:152:A:MET:HB3 | 18 | 0.28 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 10 | 0.28 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 10 | 0.28 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 10 | 0.28 |
| (1,241) | 1:70:A:ASP:HB2 | 1:74:A:ALA:H | 9 | 0.28 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 3 | 0.28 |
| (1,132) | 1:56:A:MET:HB2 | 1:57:A:THR:H | 9 | 0.28 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG11 | 1 | 0.28 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG12 | 1 | 0.28 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG13 | 1 | 0.28 |
| (1,90) | 1:185:A:VAL:HA | 1:188:A:LYS:H | 13 | 0.28 |
| (1,78) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 9 | 0.28 |
| (1,67) | 1:26:A:PHE:H | 1:59:A:TYR:H | 10 | 0.28 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 7 | 0.28 |
| (1,40) | 1:5:A:ASP:H | 1:7:A:LYS:HB2 | 12 | 0.28 |
| (1,3) | 1:152:A:MET:HB3 | 1:160:A:LEU:H | 12 | 0.28 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 9 | 0.27 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 9 | 0.27 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 9 | 0.27 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 9 | 0.27 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 9 | 0.27 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 9 | 0.27 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 11 | 0.27 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 11 | 0.27 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 11 | 0.27 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 11 | 0.27 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 10 | 0.27 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 10 | 0.27 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 10 | 0.27 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 10 | 0.27 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 10 | 0.27 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 10 | 0.27 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 8 | 0.27 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 8 | 0.27 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 19 | 0.27 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 19 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3311) | 1:29:A:TYR:HD1 | 1:71:A:LEU:HB2 | 18 | 0.27 |
| (1,3311) | 1:29:A:TYR:HD2 | 1:71:A:LEU:HB2 | 18 | 0.27 |
| (1,3287) | 1:30:A:CYS:HB3 | 1:31:A:PRO:HD3 | 5 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 5 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 5 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 5 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 5 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 5 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 5 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 5 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 5 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 5 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 8 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 8 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 8 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 8 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 8 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 8 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 8 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 8 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 8 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 9 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 9 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 9 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 9 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 9 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 9 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 9 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 9 | 0.27 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 9 | 0.27 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB1 | 6 | 0.27 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB2 | 6 | 0.27 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB3 | 6 | 0.27 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG11 | 15 | 0.27 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG12 | 15 | 0.27 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG13 | 15 | 0.27 |
| (1,2905) | 1:49:A:LYS:HA | 1:49:A:LYS:HD3 | 8 | 0.27 |
| (1,2905) | 1:49:A:LYS:HA | 1:49:A:LYS:HD3 | 14 | 0.27 |
| (1,2905) | 1:49:A:LYS:HA | 1:49:A:LYS:HD3 | 20 | 0.27 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 1 | 0.27 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 10 | 0.27 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 16 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 19 | 0.27 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 19 | 0.27 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 19 | 0.27 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 2 | 0.27 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 2 | 0.27 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 2 | 0.27 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 2 | 0.27 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 2 | 0.27 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 2 | 0.27 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 16 | 0.27 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 16 | 0.27 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 16 | 0.27 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 16 | 0.27 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 16 | 0.27 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 16 | 0.27 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 1 | 0.27 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 1 | 0.27 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 1 | 0.27 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 4 | 0.27 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 4 | 0.27 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 4 | 0.27 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG21 | 15 | 0.27 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG22 | 15 | 0.27 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG23 | 15 | 0.27 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG21 | 15 | 0.27 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG22 | 15 | 0.27 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG23 | 15 | 0.27 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG21 | 15 | 0.27 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG22 | 15 | 0.27 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG23 | 15 | 0.27 |
| (1,2621) | 1:101:A:VAL:HG21 | 1:106:A:ASP:H | 3 | 0.27 |
| (1,2621) | 1:101:A:VAL:HG22 | 1:106:A:ASP:H | 3 | 0.27 |
| (1,2621) | 1:101:A:VAL:HG23 | 1:106:A:ASP:H | 3 | 0.27 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 10 | 0.27 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 10 | 0.27 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 10 | 0.27 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 10 | 0.27 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 10 | 0.27 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 10 | 0.27 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 10 | 0.27 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 10 | 0.27 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 10 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG21 | 1 | 0.27 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG22 | 1 | 0.27 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG23 | 1 | 0.27 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 18 | 0.27 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 10 | 0.27 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 10 | 0.27 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 10 | 0.27 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 10 | 0.27 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 10 | 0.27 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 10 | 0.27 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 10 | 0.27 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 10 | 0.27 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 10 | 0.27 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD21 | 9 | 0.27 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD22 | 9 | 0.27 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD23 | 9 | 0.27 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 14 | 0.27 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 19 | 0.27 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 19 | 0.27 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 19 | 0.27 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 19 | 0.27 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 19 | 0.27 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 19 | 0.27 |
| (1,2393) | 1:83:A:VAL:HG11 | 1:86:A:LYS:HG2 | 7 | 0.27 |
| (1,2393) | 1:83:A:VAL:HG12 | 1:86:A:LYS:HG2 | 7 | 0.27 |
| (1,2393) | 1:83:A:VAL:HG13 | 1:86:A:LYS:HG2 | 7 | 0.27 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 2 | 0.27 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 10 | 0.27 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 15 | 0.27 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 13 | 0.27 |
| (1,2171) | 1:86:A:LYS:H | 1:87:A:ILE:HG12 | 6 | 0.27 |
| (1,2171) | 1:86:A:LYS:H | 1:87:A:ILE:HG12 | 7 | 0.27 |
| (1,2156) | 1:35:A:GLN:HG2 | 1:40:A:LEU:HG | 18 | 0.27 |
| (1,2156) | 1:35:A:GLN:HG3 | 1:40:A:LEU:HG | 18 | 0.27 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 2 | 0.27 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 6 | 0.27 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 7 | 0.27 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 12 | 0.27 |
| (1,2118) | 1:10:A:ILE:HG13 | 1:159:A:GLN:H | 1 | 0.27 |
| (1,2105) | 1:29:A:TYR:HE1 | 1:66:A:PRO:HG3 | 6 | 0.27 |
| (1,2105) | 1:29:A:TYR:HE2 | 1:66:A:PRO:HG3 | 6 | 0.27 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 18 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 19 | 0.27 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 3 | 0.27 |
| (1,1954) | 1:171:A:ASP:HB2 | 1:172:A:VAL:HA | 11 | 0.27 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 3 | 0.27 |
| (1,1930) | 1:186:A:GLU:HB3 | 1:187:A:LYS:H | 5 | 0.27 |
| (1,1930) | 1:186:A:GLU:HB3 | 1:187:A:LYS:H | 13 | 0.27 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE1 | 14 | 0.27 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE2 | 14 | 0.27 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE3 | 14 | 0.27 |
| (1,1778) | 1:72:A:THR:HB | 1:73:A:GLN:HB3 | 16 | 0.27 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 19 | 0.27 |
| (1,1694) | 1:136:A:GLN:HG2 | 1:137:A:GLN:H | 3 | 0.27 |
| (1,1694) | 1:136:A:GLN:HG2 | 1:137:A:GLN:H | 5 | 0.27 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG2 | 3 | 0.27 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG3 | 3 | 0.27 |
| (1,1565) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 12 | 0.27 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 17 | 0.27 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 17 | 0.27 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 17 | 0.27 |
| (1,1563) | 1:152:A:MET:HB3 | 1:160:A:LEU:HB3 | 17 | 0.27 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 15 | 0.27 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 15 | 0.27 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 15 | 0.27 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 19 | 0.27 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 14 | 0.27 |
| (1,1526) | 1:63:A:PHE:HB2 | 1:64:A:LEU:H | 10 | 0.27 |
| (1,1526) | 1:63:A:PHE:HB2 | 1:64:A:LEU:H | 19 | 0.27 |
| (1,1513) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB2 | 17 | 0.27 |
| (1,1513) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB2 | 17 | 0.27 |
| (1,1513) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB2 | 17 | 0.27 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 5 | 0.27 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG11 | 3 | 0.27 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG12 | 3 | 0.27 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG13 | 3 | 0.27 |
| (1,1450) | 1:42:A:VAL:HA | 1:45:A:ASN:HB3 | 16 | 0.27 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 9 | 0.27 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 9 | 0.27 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 9 | 0.27 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 13 | 0.27 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 13 | 0.27 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 13 | 0.27 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 19 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 19 | 0.27 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 19 | 0.27 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB2 | 18 | 0.27 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB3 | 18 | 0.27 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG11 | 19 | 0.27 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG12 | 19 | 0.27 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG13 | 19 | 0.27 |
| (1,1164) | 1:27:A:SER:H | 1:30:A:CYS:HB3 | 16 | 0.27 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 1 | 0.27 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 6 | 0.27 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 15 | 0.27 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 17 | 0.27 |
| (1,1040) | 1:52:A:GLU:HB3 | 1:53:A:GLY:H | 9 | 0.27 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 13 | 0.27 |
| (1,1005) | 1:46:A:VAL:HG21 | 1:48:A:GLN:H | 2 | 0.27 |
| (1,1005) | 1:46:A:VAL:HG22 | 1:48:A:GLN:H | 2 | 0.27 |
| (1,1005) | 1:46:A:VAL:HG23 | 1:48:A:GLN:H | 2 | 0.27 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 16 | 0.27 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 10 | 0.27 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 10 | 0.27 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 10 | 0.27 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 5 | 0.27 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 19 | 0.27 |
| (1,883) | 1:49:A:LYS:H | 1:49:A:LYS:HD3 | 18 | 0.27 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 1 | 0.27 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 1 | 0.27 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 1 | 0.27 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 11 | 0.27 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 11 | 0.27 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 11 | 0.27 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 15 | 0.27 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 15 | 0.27 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 15 | 0.27 |
| (1,799) | 1:49:A:LYS:HG2 | 1:179:A:ASP:H | 3 | 0.27 |
| (1,799) | 1:49:A:LYS:HG3 | 1:179:A:ASP:H | 3 | 0.27 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 6 | 0.27 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 5 | 0.27 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 4 | 0.27 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 2 | 0.27 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 15 | 0.27 |
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 4 | 0.27 |
| (1,614) | 1:10:A:ILE:H | 1:184:A:LEU:HD21 | 5 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,614) | 1:10:A:ILE:H | 1:184:A:LEU:HD22 | 5 | 0.27 |
| (1,614) | 1:10:A:ILE:H | 1:184:A:LEU:HD23 | 5 | 0.27 |
| (1,555) | 1:174:A:VAL:HG21 | 1:178:A:ALA:H | 17 | 0.27 |
| (1,555) | 1:174:A:VAL:HG22 | 1:178:A:ALA:H | 17 | 0.27 |
| (1,555) | 1:174:A:VAL:HG23 | 1:178:A:ALA:H | 17 | 0.27 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 9 | 0.27 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 9 | 0.27 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 9 | 0.27 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 2 | 0.27 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 2 | 0.27 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 2 | 0.27 |
| (1,498) | 1:77:A:VAL:HG11 | 1:124:A:ALA:H | 6 | 0.27 |
| (1,498) | 1:77:A:VAL:HG12 | 1:124:A:ALA:H | 6 | 0.27 |
| (1,498) | 1:77:A:VAL:HG13 | 1:124:A:ALA:H | 6 | 0.27 |
| (1,492) | 1:138:A:GLU:HB2 | 1:140:A:ALA:H | 13 | 0.27 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 18 | 0.27 |
| (1,401) | 1:117:A:LYS:HB2 | 1:120:A:ASP:H | 9 | 0.27 |
| (1,380) | 1:138:A:GLU:H | 1:138:A:GLU:HG3 | 17 | 0.27 |
| (1,315) | 1:154:A:VAL:H | 1:158:A:TYR:HB3 | 8 | 0.27 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 13 | 0.27 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 13 | 0.27 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 13 | 0.27 |
| (1,241) | 1:70:A:ASP:HB2 | 1:74:A:ALA:H | 13 | 0.27 |
| (1,241) | 1:70:A:ASP:HB2 | 1:74:A:ALA:H | 19 | 0.27 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 13 | 0.27 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 15 | 0.27 |
| (1,127) | 1:105:A:ALA:H | 1:107:A:ILE:HB | 8 | 0.27 |
| (1,111) | 1:103:A:SER:HB2 | 1:105:A:ALA:H | 6 | 0.27 |
| (1,78) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 1 | 0.27 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 5 | 0.27 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 18 | 0.27 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 15 | 0.26 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 15 | 0.26 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 15 | 0.26 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 15 | 0.26 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 15 | 0.26 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 15 | 0.26 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 1 | 0.26 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 1 | 0.26 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 4 | 0.26 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 4 | 0.26 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 5 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 3 | 0.26 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 3 | 0.26 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 10 | 0.26 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 10 | 0.26 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 10 | 0.26 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 10 | 0.26 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 10 | 0.26 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 10 | 0.26 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG21 | 17 | 0.26 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG22 | 17 | 0.26 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG23 | 17 | 0.26 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG21 | 17 | 0.26 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG22 | 17 | 0.26 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG23 | 17 | 0.26 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG21 | 17 | 0.26 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG22 | 17 | 0.26 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG23 | 17 | 0.26 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 19 | 0.26 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 19 | 0.26 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 19 | 0.26 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 19 | 0.26 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 19 | 0.26 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 19 | 0.26 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 19 | 0.26 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 19 | 0.26 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 19 | 0.26 |
| (1,2974) | 1:77:A:VAL:HG11 | 1:124:A:ALA:HB1 | 9 | 0.26 |
| (1,2974) | 1:77:A:VAL:HG11 | 1:124:A:ALA:HB2 | 9 | 0.26 |
| (1,2974) | 1:77:A:VAL:HG11 | 1:124:A:ALA:HB3 | 9 | 0.26 |
| (1,2974) | 1:77:A:VAL:HG12 | 1:124:A:ALA:HB1 | 9 | 0.26 |
| (1,2974) | 1:77:A:VAL:HG12 | 1:124:A:ALA:HB2 | 9 | 0.26 |
| (1,2974) | 1:77:A:VAL:HG12 | 1:124:A:ALA:HB3 | 9 | 0.26 |
| (1,2974) | 1:77:A:VAL:HG13 | 1:124:A:ALA:HB1 | 9 | 0.26 |
| (1,2974) | 1:77:A:VAL:HG13 | 1:124:A:ALA:HB2 | 9 | 0.26 |
| (1,2974) | 1:77:A:VAL:HG13 | 1:124:A:ALA:HB3 | 9 | 0.26 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG11 | 19 | 0.26 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG12 | 19 | 0.26 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG13 | 19 | 0.26 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 3 | 0.26 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 19 | 0.26 |
| (1,2846) | 1:2:A:GLN:HA | 1:183:A:GLN:HE22 | 10 | 0.26 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 10 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 10 | 0.26 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 10 | 0.26 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 16 | 0.26 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 16 | 0.26 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 16 | 0.26 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 2 | 0.26 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 13 | 0.26 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 13 | 0.26 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 13 | 0.26 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 13 | 0.26 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 13 | 0.26 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 13 | 0.26 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 13 | 0.26 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 13 | 0.26 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 13 | 0.26 |
| (1,2753) | 1:61:A:VAL:HG11 | 1:62:A:GLU:HA | 6 | 0.26 |
| (1,2753) | 1:61:A:VAL:HG12 | 1:62:A:GLU:HA | 6 | 0.26 |
| (1,2753) | 1:61:A:VAL:HG13 | 1:62:A:GLU:HA | 6 | 0.26 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 5 | 0.26 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 5 | 0.26 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 5 | 0.26 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 5 | 0.26 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 5 | 0.26 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 5 | 0.26 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG21 | 2 | 0.26 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG22 | 2 | 0.26 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG23 | 2 | 0.26 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG21 | 2 | 0.26 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG22 | 2 | 0.26 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG23 | 2 | 0.26 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG21 | 2 | 0.26 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG22 | 2 | 0.26 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG23 | 2 | 0.26 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG21 | 14 | 0.26 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG22 | 14 | 0.26 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG23 | 14 | 0.26 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG21 | 14 | 0.26 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG22 | 14 | 0.26 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG23 | 14 | 0.26 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG21 | 14 | 0.26 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG22 | 14 | 0.26 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG23 | 14 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2632) | 1:101:A:VAL:HG21 | 1:107:A:ILE:H | 9 | 0.26 |
| (1,2632) | 1:101:A:VAL:HG22 | 1:107:A:ILE:H | 9 | 0.26 |
| (1,2632) | 1:101:A:VAL:HG23 | 1:107:A:ILE:H | 9 | 0.26 |
| (1,2622) | 1:149:A:VAL:HA | 1:151:A:ALA:H | 5 | 0.26 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 16 | 0.26 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 16 | 0.26 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 16 | 0.26 |
| (1,2588) | 1:70:A:ASP:HA | 1:72:A:THR:H | 3 | 0.26 |
| (1,2588) | 1:70:A:ASP:HA | 1:72:A:THR:H | 15 | 0.26 |
| (1,2563) | 1:96:A:GLN:HA | 1:96:A:GLN:HE22 | 7 | 0.26 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG21 | 17 | 0.26 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG22 | 17 | 0.26 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG23 | 17 | 0.26 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG21 | 17 | 0.26 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG22 | 17 | 0.26 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG23 | 17 | 0.26 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG21 | 17 | 0.26 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG22 | 17 | 0.26 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG23 | 17 | 0.26 |
| (1,2474) | 1:83:A:VAL:HA | 1:84:A:GLU:HB2 | 11 | 0.26 |
| (1,2408) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HA | 12 | 0.26 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 4 | 0.26 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 18 | 0.26 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 18 | 0.26 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 18 | 0.26 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 18 | 0.26 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 18 | 0.26 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 18 | 0.26 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 7 | 0.26 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 5 | 0.26 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 7 | 0.26 |
| (1,2172) | 1:79:A:ILE:HG12 | 1:80:A:ALA:H | 8 | 0.26 |
| (1,2166) | 1:8:A:GLN:HB3 | 1:180:A:THR:HG21 | 19 | 0.26 |
| (1,2166) | 1:8:A:GLN:HB3 | 1:180:A:THR:HG22 | 19 | 0.26 |
| (1,2166) | 1:8:A:GLN:HB3 | 1:180:A:THR:HG23 | 19 | 0.26 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 20 | 0.26 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 16 | 0.26 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 17 | 0.26 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 9 | 0.26 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 16 | 0.26 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD1 | 15 | 0.26 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD2 | 15 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 11 | 0.26 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 16 | 0.26 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 16 | 0.26 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 16 | 0.26 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 17 | 0.26 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD1 | 12 | 0.26 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD2 | 12 | 0.26 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE1 | 9 | 0.26 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE2 | 9 | 0.26 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE3 | 9 | 0.26 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG12 | 19 | 0.26 |
| (1,1757) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HG13 | 19 | 0.26 |
| (1,1699) | 1:135:A:ALA:HB1 | 1:136:A:GLN:HG2 | 5 | 0.26 |
| (1,1699) | 1:135:A:ALA:HB2 | 1:136:A:GLN:HG2 | 5 | 0.26 |
| (1,1699) | 1:135:A:ALA:HB3 | 1:136:A:GLN:HG2 | 5 | 0.26 |
| (1,1698) | 1:136:A:GLN:HB2 | 1:136:A:GLN:HG2 | 17 | 0.26 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 3 | 0.26 |
| (1,1694) | 1:136:A:GLN:HG2 | 1:137:A:GLN:H | 4 | 0.26 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG2 | 4 | 0.26 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG3 | 4 | 0.26 |
| (1,1669) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HG2 | 7 | 0.26 |
| (1,1669) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HG2 | 7 | 0.26 |
| (1,1669) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HG2 | 7 | 0.26 |
| (1,1579) | 1:117:A:LYS:HG3 | 1:119:A:GLU:HG2 | 8 | 0.26 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 6 | 0.26 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 6 | 0.26 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 6 | 0.26 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 17 | 0.26 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 17 | 0.26 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 17 | 0.26 |
| (1,1526) | 1:63:A:PHE:HB2 | 1:64:A:LEU:H | 8 | 0.26 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 20 | 0.26 |
| (1,1474) | 1:161:A:ASN:HB2 | 1:161:A:ASN:HD22 | 20 | 0.26 |
| (1,1438) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HB2 | 5 | 0.26 |
| (1,1438) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HB2 | 5 | 0.26 |
| (1,1438) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HB2 | 5 | 0.26 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE2 | 3 | 0.26 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE3 | 3 | 0.26 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE2 | 3 | 0.26 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE3 | 3 | 0.26 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE2 | 3 | 0.26 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE3 | 3 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 4 | 0.26 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 4 | 0.26 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 4 | 0.26 |
| (1,1258) | 1:163:A:GLN:HG2 | 1:164:A:GLY:HA3 | 12 | 0.26 |
| (1,1258) | 1:163:A:GLN:HG3 | 1:164:A:GLY:HA3 | 12 | 0.26 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 2 | 0.26 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 1 | 0.26 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 1 | 0.26 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 1 | 0.26 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 11 | 0.26 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 15 | 0.26 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD21 | 18 | 0.26 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD22 | 18 | 0.26 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD23 | 18 | 0.26 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 20 | 0.26 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 1 | 0.26 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 11 | 0.26 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 11 | 0.26 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 11 | 0.26 |
| (1,730) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 18 | 0.26 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 9 | 0.26 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 14 | 0.26 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 18 | 0.26 |
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 5 | 0.26 |
| (1,606) | 1:137:A:GLN:H | 1:137:A:GLN:HG2 | 9 | 0.26 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 3 | 0.26 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 3 | 0.26 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 3 | 0.26 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 2 | 0.26 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 2 | 0.26 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 2 | 0.26 |
| (1,485) | 1:4:A:THR:H | 1:7:A:LYS:HB2 | 4 | 0.26 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 5 | 0.26 |
| (1,453) | 1:40:A:LEU:HD21 | 1:171:A:ASP:H | 18 | 0.26 |
| (1,453) | 1:40:A:LEU:HD22 | 1:171:A:ASP:H | 18 | 0.26 |
| (1,453) | 1:40:A:LEU:HD23 | 1:171:A:ASP:H | 18 | 0.26 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD11 | 4 | 0.26 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD12 | 4 | 0.26 |
| (1,303) | 1:154:A:VAL:H | 1:160:A:LEU:HD13 | 4 | 0.26 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 13 | 0.26 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG11 | 17 | 0.26 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG12 | 17 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG13 | 17 | 0.26 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE1 | 1 | 0.25 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE2 | 1 | 0.25 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE1 | 1 | 0.25 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE2 | 1 | 0.25 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE1 | 1 | 0.25 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE2 | 1 | 0.25 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 20 | 0.25 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 20 | 0.25 |
| (1,3420) | 1:60:A:HIS:HB3 | 1:75:A:TRP:HD1 | 2 | 0.25 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD1 | 16 | 0.25 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD2 | 16 | 0.25 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB2 | 14 | 0.25 |
| (1,3299) | 1:23:A:LEU:HB2 | 1:153:A:TYR:HB3 | 14 | 0.25 |
| (1,3269) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA2 | 14 | 0.25 |
| (1,3269) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA2 | 14 | 0.25 |
| (1,3269) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA2 | 14 | 0.25 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 5 | 0.25 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 13 | 0.25 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 10 | 0.25 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 10 | 0.25 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 10 | 0.25 |
| (1,2753) | 1:61:A:VAL:HG11 | 1:62:A:GLU:HA | 19 | 0.25 |
| (1,2753) | 1:61:A:VAL:HG12 | 1:62:A:GLU:HA | 19 | 0.25 |
| (1,2753) | 1:61:A:VAL:HG13 | 1:62:A:GLU:HA | 19 | 0.25 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG11 | 18 | 0.25 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG12 | 18 | 0.25 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG13 | 18 | 0.25 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 12 | 0.25 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 12 | 0.25 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 12 | 0.25 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 10 | 0.25 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 10 | 0.25 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 10 | 0.25 |
| (1,2622) | 1:149:A:VAL:HA | 1:151:A:ALA:H | 6 | 0.25 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 13 | 0.25 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 13 | 0.25 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 13 | 0.25 |
| (1,2581) | 1:52:A:GLU:HA | 1:53:A:GLY:HA3 | 15 | 0.25 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 12 | 0.25 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 12 | 0.25 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 12 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 12 | 0.25 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 12 | 0.25 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 12 | 0.25 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 12 | 0.25 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 12 | 0.25 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 12 | 0.25 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 11 | 0.25 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 17 | 0.25 |
| (1,2452) | 1:149:A:VAL:HG11 | 1:150:A:PRO:HG3 | 19 | 0.25 |
| (1,2452) | 1:149:A:VAL:HG12 | 1:150:A:PRO:HG3 | 19 | 0.25 |
| (1,2452) | 1:149:A:VAL:HG13 | 1:150:A:PRO:HG3 | 19 | 0.25 |
| (1,2452) | 1:149:A:VAL:HG21 | 1:150:A:PRO:HG3 | 19 | 0.25 |
| (1,2452) | 1:149:A:VAL:HG22 | 1:150:A:PRO:HG3 | 19 | 0.25 |
| (1,2452) | 1:149:A:VAL:HG23 | 1:150:A:PRO:HG3 | 19 | 0.25 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 5 | 0.25 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 16 | 0.25 |
| (1,2316) | 1:117:A:LYS:H | 1:117:A:LYS:HG2 | 20 | 0.25 |
| (1,2291) | 1:117:A:LYS:HG3 | 1:120:A:ASP:H | 11 | 0.25 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 12 | 0.25 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 12 | 0.25 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 12 | 0.25 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 12 | 0.25 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 12 | 0.25 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 12 | 0.25 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 19 | 0.25 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 6 | 0.25 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 3 | 0.25 |
| (1,2046) | 1:119:A:GLU:H | 1:119:A:GLU:HB2 | 4 | 0.25 |
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 17 | 0.25 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 7 | 0.25 |
| (1,1938) | 1:184:A:LEU:H | 1:185:A:VAL:HA | 8 | 0.25 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 6 | 0.25 |
| (1,1935) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HA | 11 | 0.25 |
| (1,1930) | 1:186:A:GLU:HB3 | 1:187:A:LYS:H | 16 | 0.25 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG21 | 3 | 0.25 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG22 | 3 | 0.25 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG23 | 3 | 0.25 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 1 | 0.25 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 1 | 0.25 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 1 | 0.25 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 11 | 0.25 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 11 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 11 | 0.25 |
| (1,1869) | 1:73:A:GLN:HG2 | 1:134:A:VAL:HG21 | 9 | 0.25 |
| (1,1869) | 1:73:A:GLN:HG2 | 1:134:A:VAL:HG22 | 9 | 0.25 |
| (1,1869) | 1:73:A:GLN:HG2 | 1:134:A:VAL:HG23 | 9 | 0.25 |
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 4 | 0.25 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE1 | 4 | 0.25 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE2 | 4 | 0.25 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE3 | 4 | 0.25 |
| (1,1744) | 1:134:A:VAL:HA | 1:137:A:GLN:HG2 | 10 | 0.25 |
| (1,1730) | 1:55:A:LYS:H | 1:55:A:LYS:HB3 | 7 | 0.25 |
| (1,1698) | 1:136:A:GLN:HB2 | 1:136:A:GLN:HG2 | 16 | 0.25 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG2 | 12 | 0.25 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG3 | 12 | 0.25 |
| (1,1606) | 1:52:A:GLU:HG2 | 1:53:A:GLY:HA3 | 1 | 0.25 |
| (1,1606) | 1:52:A:GLU:HG3 | 1:53:A:GLY:HA3 | 1 | 0.25 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 2 | 0.25 |
| (1,1565) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 6 | 0.25 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 11 | 0.25 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 19 | 0.25 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 17 | 0.25 |
| (1,1528) | 1:34:A:TYR:HB2 | 1:35:A:GLN:H | 13 | 0.25 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG21 | 14 | 0.25 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG22 | 14 | 0.25 |
| (1,1429) | 1:29:A:TYR:HB2 | 1:95:A:VAL:HG23 | 14 | 0.25 |
| (1,1426) | 1:143:A:ASP:HB2 | 1:144:A:LEU:HG | 16 | 0.25 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB2 | 3 | 0.25 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB3 | 3 | 0.25 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 4 | 0.25 |
| (1,1213) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE21 | 9 | 0.25 |
| (1,1213) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE21 | 9 | 0.25 |
| (1,1213) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE21 | 9 | 0.25 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 6 | 0.25 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 17 | 0.25 |
| (1,1164) | 1:27:A:SER:H | 1:30:A:CYS:HB3 | 8 | 0.25 |
| (1,1042) | 1:7:A:LYS:HA | 1:161:A:ASN:HD22 | 17 | 0.25 |
| (1,1040) | 1:52:A:GLU:HB3 | 1:53:A:GLY:H | 15 | 0.25 |
| (1,1040) | 1:52:A:GLU:HB3 | 1:53:A:GLY:H | 20 | 0.25 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 19 | 0.25 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 4 | 0.25 |
| (1,1005) | 1:46:A:VAL:HG21 | 1:48:A:GLN:H | 9 | 0.25 |
| (1,1005) | 1:46:A:VAL:HG22 | 1:48:A:GLN:H | 9 | 0.25 |
| (1,1005) | 1:46:A:VAL:HG23 | 1:48:A:GLN:H | 9 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1005) | 1:46:A:VAL:HG21 | 1:48:A:GLN:H | 20 | 0.25 |
| (1,1005) | 1:46:A:VAL:HG22 | 1:48:A:GLN:H | 20 | 0.25 |
| (1,1005) | 1:46:A:VAL:HG23 | 1:48:A:GLN:H | 20 | 0.25 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 9 | 0.25 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 11 | 0.25 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 11 | 0.25 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 11 | 0.25 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 13 | 0.25 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 13 | 0.25 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 13 | 0.25 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 15 | 0.25 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 15 | 0.25 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 15 | 0.25 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD21 | 13 | 0.25 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD22 | 13 | 0.25 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD23 | 13 | 0.25 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 9 | 0.25 |
| (1,781) | 1:160:A:LEU:HD21 | 1:180:A:THR:H | 1 | 0.25 |
| (1,781) | 1:160:A:LEU:HD22 | 1:180:A:THR:H | 1 | 0.25 |
| (1,781) | 1:160:A:LEU:HD23 | 1:180:A:THR:H | 1 | 0.25 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 10 | 0.25 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 12 | 0.25 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 2 | 0.25 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 5 | 0.25 |
| (1,632) | 1:87:A:ILE:HG21 | 1:91:A:MET:H | 2 | 0.25 |
| (1,632) | 1:87:A:ILE:HG22 | 1:91:A:MET:H | 2 | 0.25 |
| (1,632) | 1:87:A:ILE:HG23 | 1:91:A:MET:H | 2 | 0.25 |
| (1,632) | 1:87:A:ILE:HG21 | 1:91:A:MET:H | 14 | 0.25 |
| (1,632) | 1:87:A:ILE:HG22 | 1:91:A:MET:H | 14 | 0.25 |
| (1,632) | 1:87:A:ILE:HG23 | 1:91:A:MET:H | 14 | 0.25 |
| (1,606) | 1:137:A:GLN:H | 1:137:A:GLN:HG2 | 4 | 0.25 |
| (1,599) | 1:183:A:GLN:HB3 | 1:184:A:LEU:H | 17 | 0.25 |
| (1,577) | 1:121:A:TYR:HB2 | 1:122:A:ASP:H | 8 | 0.25 |
| (1,560) | 1:42:A:VAL:HG21 | 1:178:A:ALA:H | 3 | 0.25 |
| (1,560) | 1:42:A:VAL:HG22 | 1:178:A:ALA:H | 3 | 0.25 |
| (1,560) | 1:42:A:VAL:HG23 | 1:178:A:ALA:H | 3 | 0.25 |
| (1,560) | 1:42:A:VAL:HG21 | 1:178:A:ALA:H | 10 | 0.25 |
| (1,560) | 1:42:A:VAL:HG22 | 1:178:A:ALA:H | 10 | 0.25 |
| (1,560) | 1:42:A:VAL:HG23 | 1:178:A:ALA:H | 10 | 0.25 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 5 | 0.25 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 5 | 0.25 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 5 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,485) | 1:4:A:THR:H | 1:7:A:LYS:HB2 | 19 | 0.25 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 4 | 0.25 |
| (1,441) | 1:34:A:TYR:HE2 | 1:92:A:PHE:H | 15 | 0.25 |
| (1,337) | 1:166:A:ASP:H | 1:176:A:GLN:HE21 | 17 | 0.25 |
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 13 | 0.25 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 14 | 0.25 |
| (1,216) | 1:34:A:TYR:H | 1:96:A:GLN:HE21 | 6 | 0.25 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 18 | 0.25 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG11 | 16 | 0.25 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG12 | 16 | 0.25 |
| (1,100) | 1:73:A:GLN:H | 1:134:A:VAL:HG13 | 16 | 0.25 |
| (1,83) | 1:6:A:GLY:H | 1:11:A:THR:H | 7 | 0.25 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 9 | 0.25 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 15 | 0.25 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 2 | 0.24 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 2 | 0.24 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 2 | 0.24 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 2 | 0.24 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 2 | 0.24 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 2 | 0.24 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 13 | 0.24 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 13 | 0.24 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 13 | 0.24 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 13 | 0.24 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 13 | 0.24 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 13 | 0.24 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 15 | 0.24 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 15 | 0.24 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 14 | 0.24 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 14 | 0.24 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 19 | 0.24 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 19 | 0.24 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD1 | 3 | 0.24 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD2 | 3 | 0.24 |
| (1,3297) | 1:23:A:LEU:HB2 | 1:153:A:TYR:H | 14 | 0.24 |
| (1,3229) | 1:88:A:THR:H | 1:90:A:PRO:HD3 | 5 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 3 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 3 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 3 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 3 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 3 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 3 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 3 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 3 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 3 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 18 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 18 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 18 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 18 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 18 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 18 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 18 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 18 | 0.24 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 18 | 0.24 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG11 | 3 | 0.24 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG12 | 3 | 0.24 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG13 | 3 | 0.24 |
| (1,2935) | 1:75:A:TRP:HA | 1:78:A:ALA:HA | 8 | 0.24 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 1 | 0.24 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 1 | 0.24 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 1 | 0.24 |
| (1,2838) | 1:34:A:TYR:HE1 | 1:38:A:GLU:HA | 18 | 0.24 |
| (1,2838) | 1:34:A:TYR:HE2 | 1:38:A:GLU:HA | 18 | 0.24 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG11 | 5 | 0.24 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG12 | 5 | 0.24 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG13 | 5 | 0.24 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG11 | 16 | 0.24 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG12 | 16 | 0.24 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG13 | 16 | 0.24 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG11 | 17 | 0.24 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG12 | 17 | 0.24 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG13 | 17 | 0.24 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 11 | 0.24 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 11 | 0.24 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 11 | 0.24 |
| (1,2632) | 1:101:A:VAL:HG21 | 1:107:A:ILE:H | 14 | 0.24 |
| (1,2632) | 1:101:A:VAL:HG22 | 1:107:A:ILE:H | 14 | 0.24 |
| (1,2632) | 1:101:A:VAL:HG23 | 1:107:A:ILE:H | 14 | 0.24 |
| (1,2621) | 1:101:A:VAL:HG21 | 1:106:A:ASP:H | 14 | 0.24 |
| (1,2621) | 1:101:A:VAL:HG22 | 1:106:A:ASP:H | 14 | 0.24 |
| (1,2621) | 1:101:A:VAL:HG23 | 1:106:A:ASP:H | 14 | 0.24 |
| (1,2621) | 1:101:A:VAL:HG21 | 1:106:A:ASP:H | 15 | 0.24 |
| (1,2621) | 1:101:A:VAL:HG22 | 1:106:A:ASP:H | 15 | 0.24 |
| (1,2621) | 1:101:A:VAL:HG23 | 1:106:A:ASP:H | 15 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 19 | 0.24 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 19 | 0.24 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 19 | 0.24 |
| (1,2588) | 1:70:A:ASP:HA | 1:72:A:THR:H | 19 | 0.24 |
| (1,2581) | 1:52:A:GLU:HA | 1:53:A:GLY:HA3 | 1 | 0.24 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 19 | 0.24 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 19 | 0.24 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 19 | 0.24 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 19 | 0.24 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 19 | 0.24 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 19 | 0.24 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 19 | 0.24 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 19 | 0.24 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 19 | 0.24 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 15 | 0.24 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 15 | 0.24 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 15 | 0.24 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE1 | 8 | 0.24 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE2 | 8 | 0.24 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE1 | 8 | 0.24 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE2 | 8 | 0.24 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE1 | 8 | 0.24 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE2 | 8 | 0.24 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 12 | 0.24 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 16 | 0.24 |
| (1,2304) | 1:132:A:SER:HA | 1:136:A:GLN:HG2 | 15 | 0.24 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 19 | 0.24 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 19 | 0.24 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 19 | 0.24 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 19 | 0.24 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 19 | 0.24 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 19 | 0.24 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 15 | 0.24 |
| (1,2220) | 1:67:A:LEU:HD11 | 1:103:A:SER:HB2 | 1 | 0.24 |
| (1,2220) | 1:67:A:LEU:HD12 | 1:103:A:SER:HB2 | 1 | 0.24 |
| (1,2220) | 1:67:A:LEU:HD13 | 1:103:A:SER:HB2 | 1 | 0.24 |
| (1,2220) | 1:67:A:LEU:HD11 | 1:103:A:SER:HB2 | 5 | 0.24 |
| (1,2220) | 1:67:A:LEU:HD12 | 1:103:A:SER:HB2 | 5 | 0.24 |
| (1,2220) | 1:67:A:LEU:HD13 | 1:103:A:SER:HB2 | 5 | 0.24 |
| (1,2171) | 1:86:A:LYS:H | 1:87:A:ILE:HG12 | 10 | 0.24 |
| (1,2159) | 1:76:A:ALA:HA | 1:79:A:ILE:HG12 | 7 | 0.24 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 13 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 13 | 0.24 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 13 | 0.24 |
| (1,2117) | 1:10:A:ILE:HG13 | 1:159:A:GLN:HB2 | 18 | 0.24 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG21 | 5 | 0.24 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG22 | 5 | 0.24 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG23 | 5 | 0.24 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG21 | 5 | 0.24 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG22 | 5 | 0.24 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG23 | 5 | 0.24 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB2 | 2 | 0.24 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB3 | 2 | 0.24 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 18 | 0.24 |
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 1 | 0.24 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 4 | 0.24 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 12 | 0.24 |
| (1,1931) | 1:62:A:GLU:HB2 | 1:63:A:PHE:HB3 | 1 | 0.24 |
| (1,1931) | 1:62:A:GLU:HB3 | 1:63:A:PHE:HB3 | 1 | 0.24 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 4 | 0.24 |
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 4 | 0.24 |
| (1,1832) | 1:124:A:ALA:HB1 | 1:130:A:VAL:HB | 18 | 0.24 |
| (1,1832) | 1:124:A:ALA:HB2 | 1:130:A:VAL:HB | 18 | 0.24 |
| (1,1832) | 1:124:A:ALA:HB3 | 1:130:A:VAL:HB | 18 | 0.24 |
| (1,1813) | 1:160:A:LEU:HD21 | 1:180:A:THR:HB | 9 | 0.24 |
| (1,1813) | 1:160:A:LEU:HD22 | 1:180:A:THR:HB | 9 | 0.24 |
| (1,1813) | 1:160:A:LEU:HD23 | 1:180:A:THR:HB | 9 | 0.24 |
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 10 | 0.24 |
| (1,1792) | 1:56:A:MET:HB2 | 1:56:A:MET:HG3 | 9 | 0.24 |
| (1,1785) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD2 | 1 | 0.24 |
| (1,1785) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD2 | 16 | 0.24 |
| (1,1703) | 1:59:A:TYR:HE1 | 1:136:A:GLN:HG3 | 20 | 0.24 |
| (1,1703) | 1:59:A:TYR:HE2 | 1:136:A:GLN:HG3 | 20 | 0.24 |
| (1,1699) | 1:135:A:ALA:HB1 | 1:136:A:GLN:HG2 | 3 | 0.24 |
| (1,1699) | 1:135:A:ALA:HB2 | 1:136:A:GLN:HG2 | 3 | 0.24 |
| (1,1699) | 1:135:A:ALA:HB3 | 1:136:A:GLN:HG2 | 3 | 0.24 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 3 | 0.24 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 7 | 0.24 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 8 | 0.24 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 20 | 0.24 |
| (1,1669) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HG2 | 19 | 0.24 |
| (1,1669) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HG2 | 19 | 0.24 |
| (1,1669) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HG2 | 19 | 0.24 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 20 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 13 | 0.24 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 13 | 0.24 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 14 | 0.24 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 14 | 0.24 |
| (1,1604) | 1:61:A:VAL:HA | 1:62:A:GLU:HG2 | 8 | 0.24 |
| (1,1604) | 1:61:A:VAL:HA | 1:62:A:GLU:HG2 | 20 | 0.24 |
| (1,1603) | 1:62:A:GLU:HG2 | 1:63:A:PHE:H | 18 | 0.24 |
| (1,1601) | 1:4:A:THR:HB | 1:5:A:ASP:H | 7 | 0.24 |
| (1,1565) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 20 | 0.24 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 14 | 0.24 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 14 | 0.24 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 14 | 0.24 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 5 | 0.24 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 10 | 0.24 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 15 | 0.24 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 17 | 0.24 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 18 | 0.24 |
| (1,1545) | 1:186:A:GLU:HG3 | 1:187:A:LYS:HD3 | 1 | 0.24 |
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 17 | 0.24 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 17 | 0.24 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 17 | 0.24 |
| (1,1526) | 1:63:A:PHE:HB2 | 1:64:A:LEU:H | 18 | 0.24 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 7 | 0.24 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 7 | 0.24 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 7 | 0.24 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG11 | 8 | 0.24 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG12 | 8 | 0.24 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG13 | 8 | 0.24 |
| (1,1258) | 1:163:A:GLN:HG2 | 1:164:A:GLY:HA3 | 13 | 0.24 |
| (1,1258) | 1:163:A:GLN:HG3 | 1:164:A:GLY:HA3 | 13 | 0.24 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 7 | 0.24 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 3 | 0.24 |
| (1,1150) | 1:172:A:VAL:HG21 | 1:176:A:GLN:HE21 | 18 | 0.24 |
| (1,1150) | 1:172:A:VAL:HG22 | 1:176:A:GLN:HE21 | 18 | 0.24 |
| (1,1150) | 1:172:A:VAL:HG23 | 1:176:A:GLN:HE21 | 18 | 0.24 |
| (1,1080) | 1:34:A:TYR:HD1 | 1:38:A:GLU:H | 12 | 0.24 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 20 | 0.24 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 5 | 0.24 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 17 | 0.24 |
| (1,1005) | 1:46:A:VAL:HG21 | 1:48:A:GLN:H | 6 | 0.24 |
| (1,1005) | 1:46:A:VAL:HG22 | 1:48:A:GLN:H | 6 | 0.24 |
| (1,1005) | 1:46:A:VAL:HG23 | 1:48:A:GLN:H | 6 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 12 | 0.24 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 19 | 0.24 |
| (1,938) | 1:112:A:VAL:HG11 | 1:118:A:GLY:H | 11 | 0.24 |
| (1,938) | 1:112:A:VAL:HG12 | 1:118:A:GLY:H | 11 | 0.24 |
| (1,938) | 1:112:A:VAL:HG13 | 1:118:A:GLY:H | 11 | 0.24 |
| (1,936) | 1:117:A:LYS:HG3 | 1:118:A:GLY:H | 11 | 0.24 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 3 | 0.24 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 3 | 0.24 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 3 | 0.24 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 8 | 0.24 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 8 | 0.24 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 8 | 0.24 |
| (1,883) | 1:49:A:LYS:H | 1:49:A:LYS:HD3 | 1 | 0.24 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD21 | 7 | 0.24 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD22 | 7 | 0.24 |
| (1,864) | 1:141:A:ALA:H | 1:146:A:LEU:HD23 | 7 | 0.24 |
| (1,833) | 1:42:A:VAL:HG11 | 1:174:A:VAL:H | 9 | 0.24 |
| (1,833) | 1:42:A:VAL:HG12 | 1:174:A:VAL:H | 9 | 0.24 |
| (1,833) | 1:42:A:VAL:HG13 | 1:174:A:VAL:H | 9 | 0.24 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD21 | 17 | 0.24 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD22 | 17 | 0.24 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD23 | 17 | 0.24 |
| (1,799) | 1:49:A:LYS:HG2 | 1:179:A:ASP:H | 7 | 0.24 |
| (1,799) | 1:49:A:LYS:HG3 | 1:179:A:ASP:H | 7 | 0.24 |
| (1,787) | 1:169:A:ASN:H | 1:171:A:ASP:H | 18 | 0.24 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 3 | 0.24 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 19 | 0.24 |
| (1,650) | 1:145:A:GLN:HA | 1:146:A:LEU:H | 6 | 0.24 |
| (1,650) | 1:145:A:GLN:HA | 1:146:A:LEU:H | 11 | 0.24 |
| (1,650) | 1:145:A:GLN:HA | 1:146:A:LEU:H | 12 | 0.24 |
| (1,650) | 1:145:A:GLN:HA | 1:146:A:LEU:H | 20 | 0.24 |
| (1,587) | 1:46:A:VAL:HG21 | 1:47:A:ARG:H | 4 | 0.24 |
| (1,587) | 1:46:A:VAL:HG22 | 1:47:A:ARG:H | 4 | 0.24 |
| (1,587) | 1:46:A:VAL:HG23 | 1:47:A:ARG:H | 4 | 0.24 |
| (1,587) | 1:46:A:VAL:HG21 | 1:47:A:ARG:H | 13 | 0.24 |
| (1,587) | 1:46:A:VAL:HG22 | 1:47:A:ARG:H | 13 | 0.24 |
| (1,587) | 1:46:A:VAL:HG23 | 1:47:A:ARG:H | 13 | 0.24 |
| (1,560) | 1:42:A:VAL:HG21 | 1:178:A:ALA:H | 14 | 0.24 |
| (1,560) | 1:42:A:VAL:HG22 | 1:178:A:ALA:H | 14 | 0.24 |
| (1,560) | 1:42:A:VAL:HG23 | 1:178:A:ALA:H | 14 | 0.24 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 4 | 0.24 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 4 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 4 | 0.24 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 7 | 0.24 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 7 | 0.24 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 7 | 0.24 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 13 | 0.24 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 13 | 0.24 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 13 | 0.24 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 16 | 0.24 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 16 | 0.24 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 16 | 0.24 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 18 | 0.24 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 18 | 0.24 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 18 | 0.24 |
| (1,498) | 1:77:A:VAL:HG11 | 1:124:A:ALA:H | 2 | 0.24 |
| (1,498) | 1:77:A:VAL:HG12 | 1:124:A:ALA:H | 2 | 0.24 |
| (1,498) | 1:77:A:VAL:HG13 | 1:124:A:ALA:H | 2 | 0.24 |
| (1,498) | 1:77:A:VAL:HG11 | 1:124:A:ALA:H | 14 | 0.24 |
| (1,498) | 1:77:A:VAL:HG12 | 1:124:A:ALA:H | 14 | 0.24 |
| (1,498) | 1:77:A:VAL:HG13 | 1:124:A:ALA:H | 14 | 0.24 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 8 | 0.24 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 8 | 0.24 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 8 | 0.24 |
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 1 | 0.24 |
| (1,260) | 1:70:A:ASP:H | 1:71:A:LEU:HB3 | 11 | 0.24 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 4 | 0.24 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 17 | 0.24 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 6 | 0.24 |
| (1,216) | 1:34:A:TYR:H | 1:96:A:GLN:HE21 | 13 | 0.24 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD21 | 1 | 0.24 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD22 | 1 | 0.24 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD23 | 1 | 0.24 |
| (1,78) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 5 | 0.24 |
| (1,78) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 14 | 0.24 |
| (1,78) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 20 | 0.24 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 10 | 0.24 |
| (1,40) | 1:5:A:ASP:H | 1:7:A:LYS:HB2 | 8 | 0.24 |
| (1,40) | 1:5:A:ASP:H | 1:7:A:LYS:HB2 | 9 | 0.24 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 3 | 0.23 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 3 | 0.23 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 3 | 0.23 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 3 | 0.23 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 3 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 3 | 0.23 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 20 | 0.23 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 20 | 0.23 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 20 | 0.23 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 20 | 0.23 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 20 | 0.23 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 20 | 0.23 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 7 | 0.23 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 7 | 0.23 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 7 | 0.23 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 7 | 0.23 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 7 | 0.23 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 7 | 0.23 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 17 | 0.23 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 17 | 0.23 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 12 | 0.23 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 14 | 0.23 |
| (1,3415) | 1:59:A:TYR:HD1 | 1:137:A:GLN:HG3 | 16 | 0.23 |
| (1,3415) | 1:59:A:TYR:HD2 | 1:137:A:GLN:HG3 | 16 | 0.23 |
| (1,3311) | 1:29:A:TYR:HD1 | 1:71:A:LEU:HB2 | 20 | 0.23 |
| (1,3311) | 1:29:A:TYR:HD2 | 1:71:A:LEU:HB2 | 20 | 0.23 |
| (1,3277) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA3 | 14 | 0.23 |
| (1,3277) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA3 | 14 | 0.23 |
| (1,3277) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA3 | 14 | 0.23 |
| (1,3250) | 1:68:A:GLY:HA3 | 1:71:A:LEU:HB2 | 15 | 0.23 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD11 | 13 | 0.23 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD12 | 13 | 0.23 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD13 | 13 | 0.23 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD11 | 13 | 0.23 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD12 | 13 | 0.23 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD13 | 13 | 0.23 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD11 | 13 | 0.23 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD12 | 13 | 0.23 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD13 | 13 | 0.23 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG21 | 10 | 0.23 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG22 | 10 | 0.23 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG23 | 10 | 0.23 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG21 | 10 | 0.23 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG22 | 10 | 0.23 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG23 | 10 | 0.23 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG21 | 10 | 0.23 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG22 | 10 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG23 | 10 | 0.23 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB1 | 7 | 0.23 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB2 | 7 | 0.23 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB3 | 7 | 0.23 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG11 | 12 | 0.23 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG12 | 12 | 0.23 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG13 | 12 | 0.23 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 16 | 0.23 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 16 | 0.23 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 16 | 0.23 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 16 | 0.23 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 16 | 0.23 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 16 | 0.23 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 16 | 0.23 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 16 | 0.23 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 16 | 0.23 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD21 | 14 | 0.23 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD22 | 14 | 0.23 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD23 | 14 | 0.23 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD21 | 14 | 0.23 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD22 | 14 | 0.23 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD23 | 14 | 0.23 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD21 | 14 | 0.23 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD22 | 14 | 0.23 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD23 | 14 | 0.23 |
| (1,2943) | 1:3:A:ILE:HG21 | 1:8:A:GLN:HG3 | 13 | 0.23 |
| (1,2943) | 1:3:A:ILE:HG22 | 1:8:A:GLN:HG3 | 13 | 0.23 |
| (1,2943) | 1:3:A:ILE:HG23 | 1:8:A:GLN:HG3 | 13 | 0.23 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 16 | 0.23 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 16 | 0.23 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 16 | 0.23 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 9 | 0.23 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 4 | 0.23 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 4 | 0.23 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 4 | 0.23 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 20 | 0.23 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 10 | 0.23 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 10 | 0.23 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 10 | 0.23 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 10 | 0.23 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 10 | 0.23 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 10 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 10 | 0.23 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 10 | 0.23 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 10 | 0.23 |
| (1,2779) | 1:62:A:GLU:HA | 1:69:A:LYS:H | 18 | 0.23 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 11 | 0.23 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 11 | 0.23 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 11 | 0.23 |
| (1,2753) | 1:61:A:VAL:HG11 | 1:62:A:GLU:HA | 5 | 0.23 |
| (1,2753) | 1:61:A:VAL:HG12 | 1:62:A:GLU:HA | 5 | 0.23 |
| (1,2753) | 1:61:A:VAL:HG13 | 1:62:A:GLU:HA | 5 | 0.23 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 19 | 0.23 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 19 | 0.23 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 19 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG21 | 3 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG22 | 3 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG23 | 3 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG21 | 3 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG22 | 3 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG23 | 3 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG21 | 3 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG22 | 3 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG23 | 3 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG21 | 12 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG22 | 12 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG23 | 12 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG21 | 12 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG22 | 12 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG23 | 12 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG21 | 12 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG22 | 12 | 0.23 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG23 | 12 | 0.23 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 3 | 0.23 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 3 | 0.23 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 3 | 0.23 |
| (1,2622) | 1:149:A:VAL:HA | 1:151:A:ALA:H | 11 | 0.23 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 14 | 0.23 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 14 | 0.23 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 14 | 0.23 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 14 | 0.23 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 14 | 0.23 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 14 | 0.23 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 14 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 14 | 0.23 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 14 | 0.23 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG21 | 13 | 0.23 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG22 | 13 | 0.23 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG23 | 13 | 0.23 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 13 | 0.23 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 13 | 0.23 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 13 | 0.23 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 17 | 0.23 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 17 | 0.23 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 17 | 0.23 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 17 | 0.23 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 17 | 0.23 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 17 | 0.23 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 17 | 0.23 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 17 | 0.23 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 17 | 0.23 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG21 | 10 | 0.23 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG22 | 10 | 0.23 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG23 | 10 | 0.23 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG21 | 10 | 0.23 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG22 | 10 | 0.23 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG23 | 10 | 0.23 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG21 | 10 | 0.23 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG22 | 10 | 0.23 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG23 | 10 | 0.23 |
| (1,2535) | 1:20:A:PRO:HG2 | 1:57:A:THR:HG21 | 17 | 0.23 |
| (1,2535) | 1:20:A:PRO:HG2 | 1:57:A:THR:HG22 | 17 | 0.23 |
| (1,2535) | 1:20:A:PRO:HG2 | 1:57:A:THR:HG23 | 17 | 0.23 |
| (1,2535) | 1:20:A:PRO:HG3 | 1:57:A:THR:HG21 | 17 | 0.23 |
| (1,2535) | 1:20:A:PRO:HG3 | 1:57:A:THR:HG22 | 17 | 0.23 |
| (1,2535) | 1:20:A:PRO:HG3 | 1:57:A:THR:HG23 | 17 | 0.23 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD21 | 7 | 0.23 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD22 | 7 | 0.23 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD23 | 7 | 0.23 |
| (1,2529) | 1:97:A:LYS:H | 1:98:A:THR:HG21 | 12 | 0.23 |
| (1,2529) | 1:97:A:LYS:H | 1:98:A:THR:HG22 | 12 | 0.23 |
| (1,2529) | 1:97:A:LYS:H | 1:98:A:THR:HG23 | 12 | 0.23 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE1 | 7 | 0.23 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE2 | 7 | 0.23 |
| (1,2507) | 1:50:A:LEU:HD21 | 1:56:A:MET:HE3 | 7 | 0.23 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE1 | 7 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE2 | 7 | 0.23 |
| (1,2507) | 1:50:A:LEU:HD22 | 1:56:A:MET:HE3 | 7 | 0.23 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE1 | 7 | 0.23 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE2 | 7 | 0.23 |
| (1,2507) | 1:50:A:LEU:HD23 | 1:56:A:MET:HE3 | 7 | 0.23 |
| (1,2479) | 1:8:A:GLN:HA | 1:8:A:GLN:HG2 | 9 | 0.23 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE1 | 4 | 0.23 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE2 | 4 | 0.23 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE1 | 4 | 0.23 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE2 | 4 | 0.23 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE1 | 4 | 0.23 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE2 | 4 | 0.23 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 6 | 0.23 |
| (1,2315) | 1:46:A:VAL:HG21 | 1:50:A:LEU:HG | 1 | 0.23 |
| (1,2315) | 1:46:A:VAL:HG22 | 1:50:A:LEU:HG | 1 | 0.23 |
| (1,2315) | 1:46:A:VAL:HG23 | 1:50:A:LEU:HG | 1 | 0.23 |
| (1,2279) | 1:73:A:GLN:HG3 | 1:125:A:TRP:HA | 13 | 0.23 |
| (1,2168) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HG2 | 5 | 0.23 |
| (1,2168) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HG2 | 5 | 0.23 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 15 | 0.23 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 16 | 0.23 |
| (1,2118) | 1:10:A:ILE:HG13 | 1:159:A:GLN:H | 2 | 0.23 |
| (1,2118) | 1:10:A:ILE:HG13 | 1:159:A:GLN:H | 7 | 0.23 |
| (1,2072) | 1:93:A:GLU:HA | 1:97:A:LYS:HD2 | 20 | 0.23 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 3 | 0.23 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG11 | 18 | 0.23 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG12 | 18 | 0.23 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG13 | 18 | 0.23 |
| (1,2010) | 1:48:A:GLN:H | 1:48:A:GLN:HB3 | 7 | 0.23 |
| (1,1987) | 1:79:A:ILE:HD11 | 1:136:A:GLN:HB2 | 4 | 0.23 |
| (1,1987) | 1:79:A:ILE:HD12 | 1:136:A:GLN:HB2 | 4 | 0.23 |
| (1,1987) | 1:79:A:ILE:HD13 | 1:136:A:GLN:HB2 | 4 | 0.23 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 1 | 0.23 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 16 | 0.23 |
| (1,1930) | 1:186:A:GLU:HB3 | 1:187:A:LYS:H | 3 | 0.23 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB2 | 15 | 0.23 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB3 | 15 | 0.23 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB2 | 15 | 0.23 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB3 | 15 | 0.23 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB2 | 15 | 0.23 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB3 | 15 | 0.23 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 13 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 13 | 0.23 |
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 13 | 0.23 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD1 | 20 | 0.23 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD2 | 20 | 0.23 |
| (1,1792) | 1:56:A:MET:HB2 | 1:56:A:MET:HG3 | 15 | 0.23 |
| (1,1697) | 1:132:A:SER:HB2 | 1:136:A:GLN:HG2 | 3 | 0.23 |
| (1,1697) | 1:132:A:SER:HB3 | 1:136:A:GLN:HG2 | 3 | 0.23 |
| (1,1686) | 1:99:A:GLN:HG3 | 1:100:A:THR:H | 13 | 0.23 |
| (1,1685) | 1:99:A:GLN:HA | 1:99:A:GLN:HG3 | 2 | 0.23 |
| (1,1685) | 1:99:A:GLN:HA | 1:99:A:GLN:HG3 | 16 | 0.23 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG2 | 7 | 0.23 |
| (1,1677) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HG3 | 7 | 0.23 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 11 | 0.23 |
| (1,1632) | 1:31:A:PRO:HA | 1:96:A:GLN:HG2 | 19 | 0.23 |
| (1,1628) | 1:20:A:PRO:HB2 | 1:57:A:THR:HB | 19 | 0.23 |
| (1,1628) | 1:20:A:PRO:HB3 | 1:57:A:THR:HB | 19 | 0.23 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB2 | 7 | 0.23 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB3 | 7 | 0.23 |
| (1,1608) | 1:78:A:ALA:HA | 1:84:A:GLU:HG2 | 7 | 0.23 |
| (1,1604) | 1:61:A:VAL:HA | 1:62:A:GLU:HG2 | 4 | 0.23 |
| (1,1604) | 1:61:A:VAL:HA | 1:62:A:GLU:HG2 | 7 | 0.23 |
| (1,1604) | 1:61:A:VAL:HA | 1:62:A:GLU:HG2 | 18 | 0.23 |
| (1,1603) | 1:62:A:GLU:HG2 | 1:63:A:PHE:H | 13 | 0.23 |
| (1,1565) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 18 | 0.23 |
| (1,1565) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 19 | 0.23 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 1 | 0.23 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 6 | 0.23 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 12 | 0.23 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 13 | 0.23 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 14 | 0.23 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 16 | 0.23 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 20 | 0.23 |
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 5 | 0.23 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 5 | 0.23 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 5 | 0.23 |
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 16 | 0.23 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 16 | 0.23 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 16 | 0.23 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG11 | 15 | 0.23 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG12 | 15 | 0.23 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG13 | 15 | 0.23 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG11 | 5 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG12 | 5 | 0.23 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG13 | 5 | 0.23 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 10 | 0.23 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 10 | 0.23 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 10 | 0.23 |
| (1,1438) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HB2 | 20 | 0.23 |
| (1,1438) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HB2 | 20 | 0.23 |
| (1,1438) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HB2 | 20 | 0.23 |
| (1,1432) | 1:85:A:ASP:HB3 | 1:86:A:LYS:HG2 | 5 | 0.23 |
| (1,1381) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 14 | 0.23 |
| (1,1233) | 1:147:A:GLN:HB3 | 1:148:A:GLY:H | 11 | 0.23 |
| (1,1203) | 1:30:A:CYS:H | 1:96:A:GLN:HE22 | 18 | 0.23 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 10 | 0.23 |
| (1,1198) | 1:99:A:GLN:HB3 | 1:100:A:THR:H | 11 | 0.23 |
| (1,1191) | 1:64:A:LEU:HD11 | 1:65:A:GLY:H | 9 | 0.23 |
| (1,1191) | 1:64:A:LEU:HD12 | 1:65:A:GLY:H | 9 | 0.23 |
| (1,1191) | 1:64:A:LEU:HD13 | 1:65:A:GLY:H | 9 | 0.23 |
| (1,1040) | 1:52:A:GLU:HB3 | 1:53:A:GLY:H | 4 | 0.23 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 12 | 0.23 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 18 | 0.23 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 19 | 0.23 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 1 | 0.23 |
| (1,967) | 1:126:A:ASN:HB2 | 1:126:A:ASN:HD22 | 1 | 0.23 |
| (1,967) | 1:126:A:ASN:HB2 | 1:126:A:ASN:HD22 | 13 | 0.23 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 20 | 0.23 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 20 | 0.23 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 20 | 0.23 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 8 | 0.23 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 8 | 0.23 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 8 | 0.23 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD21 | 5 | 0.23 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD22 | 5 | 0.23 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD23 | 5 | 0.23 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 20 | 0.23 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 11 | 0.23 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 14 | 0.23 |
| (1,745) | 1:119:A:GLU:H | 1:123:A:ALA:H | 15 | 0.23 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 20 | 0.23 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 20 | 0.23 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 20 | 0.23 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 3 | 0.23 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 4 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,645) | 1:76:A:ALA:H | 1:77:A:VAL:HG21 | 2 | 0.23 |
| (1,645) | 1:76:A:ALA:H | 1:77:A:VAL:HG22 | 2 | 0.23 |
| (1,645) | 1:76:A:ALA:H | 1:77:A:VAL:HG23 | 2 | 0.23 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 16 | 0.23 |
| (1,632) | 1:87:A:ILE:HG21 | 1:91:A:MET:H | 13 | 0.23 |
| (1,632) | 1:87:A:ILE:HG22 | 1:91:A:MET:H | 13 | 0.23 |
| (1,632) | 1:87:A:ILE:HG23 | 1:91:A:MET:H | 13 | 0.23 |
| (1,606) | 1:137:A:GLN:H | 1:137:A:GLN:HG2 | 1 | 0.23 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 2 | 0.23 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 2 | 0.23 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 2 | 0.23 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 17 | 0.23 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 17 | 0.23 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 17 | 0.23 |
| (1,568) | 1:49:A:LYS:HA | 1:50:A:LEU:H | 6 | 0.23 |
| (1,555) | 1:174:A:VAL:HG21 | 1:178:A:ALA:H | 5 | 0.23 |
| (1,555) | 1:174:A:VAL:HG22 | 1:178:A:ALA:H | 5 | 0.23 |
| (1,555) | 1:174:A:VAL:HG23 | 1:178:A:ALA:H | 5 | 0.23 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 1 | 0.23 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 1 | 0.23 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 1 | 0.23 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 17 | 0.23 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 17 | 0.23 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 17 | 0.23 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 19 | 0.23 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 19 | 0.23 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 19 | 0.23 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD11 | 5 | 0.23 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD12 | 5 | 0.23 |
| (1,514) | 1:26:A:PHE:H | 1:146:A:LEU:HD13 | 5 | 0.23 |
| (1,485) | 1:4:A:THR:H | 1:7:A:LYS:HB2 | 15 | 0.23 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 10 | 0.23 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 10 | 0.23 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 10 | 0.23 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 16 | 0.23 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 16 | 0.23 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 16 | 0.23 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 4 | 0.23 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 4 | 0.23 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 4 | 0.23 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 19 | 0.23 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 19 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 19 | 0.23 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 9 | 0.23 |
| (1,132) | 1:56:A:MET:HB2 | 1:57:A:THR:H | 1 | 0.23 |
| (1,132) | 1:56:A:MET:HB2 | 1:57:A:THR:H | 6 | 0.23 |
| (1,90) | 1:185:A:VAL:HA | 1:188:A:LYS:H | 19 | 0.23 |
| (1,83) | 1:6:A:GLY:H | 1:11:A:THR:H | 17 | 0.23 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 6 | 0.23 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 12 | 0.23 |
| (1,3) | 1:152:A:MET:HB3 | 1:160:A:LEU:H | 15 | 0.23 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE1 | 12 | 0.22 |
| (1,3522) | 1:152:A:MET:HE1 | 1:177:A:TYR:HE2 | 12 | 0.22 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE1 | 12 | 0.22 |
| (1,3522) | 1:152:A:MET:HE2 | 1:177:A:TYR:HE2 | 12 | 0.22 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE1 | 12 | 0.22 |
| (1,3522) | 1:152:A:MET:HE3 | 1:177:A:TYR:HE2 | 12 | 0.22 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG2 | 18 | 0.22 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG3 | 18 | 0.22 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD1 | 6 | 0.22 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD2 | 6 | 0.22 |
| (1,3287) | 1:30:A:CYS:HB3 | 1:31:A:PRO:HD3 | 20 | 0.22 |
| (1,3276) | 1:118:A:GLY:HA3 | 1:121:A:TYR:HB3 | 5 | 0.22 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 2 | 0.22 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 2 | 0.22 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 2 | 0.22 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 2 | 0.22 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 2 | 0.22 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 2 | 0.22 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 2 | 0.22 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 2 | 0.22 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 2 | 0.22 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 18 | 0.22 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 18 | 0.22 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 18 | 0.22 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 18 | 0.22 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 18 | 0.22 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 18 | 0.22 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 18 | 0.22 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 18 | 0.22 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 18 | 0.22 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG11 | 7 | 0.22 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG12 | 7 | 0.22 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG13 | 7 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG11 | 7 | 0.22 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG12 | 7 | 0.22 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG13 | 7 | 0.22 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG11 | 7 | 0.22 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG12 | 7 | 0.22 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG13 | 7 | 0.22 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 2 | 0.22 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 2 | 0.22 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 2 | 0.22 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 5 | 0.22 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 5 | 0.22 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 5 | 0.22 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 9 | 0.22 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 9 | 0.22 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 9 | 0.22 |
| (1,2838) | 1:34:A:TYR:HE1 | 1:38:A:GLU:HA | 13 | 0.22 |
| (1,2838) | 1:34:A:TYR:HE2 | 1:38:A:GLU:HA | 13 | 0.22 |
| (1,2753) | 1:61:A:VAL:HG11 | 1:62:A:GLU:HA | 13 | 0.22 |
| (1,2753) | 1:61:A:VAL:HG12 | 1:62:A:GLU:HA | 13 | 0.22 |
| (1,2753) | 1:61:A:VAL:HG13 | 1:62:A:GLU:HA | 13 | 0.22 |
| (1,2753) | 1:61:A:VAL:HG11 | 1:62:A:GLU:HA | 15 | 0.22 |
| (1,2753) | 1:61:A:VAL:HG12 | 1:62:A:GLU:HA | 15 | 0.22 |
| (1,2753) | 1:61:A:VAL:HG13 | 1:62:A:GLU:HA | 15 | 0.22 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG11 | 12 | 0.22 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG12 | 12 | 0.22 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG13 | 12 | 0.22 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG11 | 19 | 0.22 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG12 | 19 | 0.22 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG13 | 19 | 0.22 |
| (1,2600) | 1:37:A:GLU:HA | 1:37:A:GLU:HG2 | 13 | 0.22 |
| (1,2588) | 1:70:A:ASP:HA | 1:72:A:THR:H | 11 | 0.22 |
| (1,2588) | 1:70:A:ASP:HA | 1:72:A:THR:H | 16 | 0.22 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG11 | 7 | 0.22 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG12 | 7 | 0.22 |
| (1,2578) | 1:28:A:PHE:HB3 | 1:95:A:VAL:HG13 | 7 | 0.22 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG21 | 20 | 0.22 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG22 | 20 | 0.22 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG23 | 20 | 0.22 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 8 | 0.22 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 8 | 0.22 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 8 | 0.22 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD21 | 8 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD22 | 8 | 0.22 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD23 | 8 | 0.22 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 5 | 0.22 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 12 | 0.22 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE1 | 16 | 0.22 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE2 | 16 | 0.22 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE1 | 16 | 0.22 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE2 | 16 | 0.22 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE1 | 16 | 0.22 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE2 | 16 | 0.22 |
| (1,2315) | 1:46:A:VAL:HG21 | 1:50:A:LEU:HG | 8 | 0.22 |
| (1,2315) | 1:46:A:VAL:HG22 | 1:50:A:LEU:HG | 8 | 0.22 |
| (1,2315) | 1:46:A:VAL:HG23 | 1:50:A:LEU:HG | 8 | 0.22 |
| (1,2315) | 1:46:A:VAL:HG21 | 1:50:A:LEU:HG | 18 | 0.22 |
| (1,2315) | 1:46:A:VAL:HG22 | 1:50:A:LEU:HG | 18 | 0.22 |
| (1,2315) | 1:46:A:VAL:HG23 | 1:50:A:LEU:HG | 18 | 0.22 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG21 | 9 | 0.22 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG22 | 9 | 0.22 |
| (1,2309) | 1:132:A:SER:HA | 1:134:A:VAL:HG23 | 9 | 0.22 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 4 | 0.22 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 4 | 0.22 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 4 | 0.22 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 4 | 0.22 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 4 | 0.22 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 4 | 0.22 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 20 | 0.22 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 20 | 0.22 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 20 | 0.22 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 20 | 0.22 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 20 | 0.22 |
| (1,2118) | 1:10:A:ILE:HG13 | 1:159:A:GLN:H | 20 | 0.22 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 14 | 0.22 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 6 | 0.22 |
| (1,1981) | 1:187:A:LYS:H | 1:187:A:LYS:HD3 | 15 | 0.22 |
| (1,1981) | 1:187:A:LYS:H | 1:187:A:LYS:HD3 | 20 | 0.22 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 1 | 0.22 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 18 | 0.22 |
| (1,1935) | 1:128:A:PHE:HB3 | 1:129:A:VAL:HA | 5 | 0.22 |
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 1 | 0.22 |
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 3 | 0.22 |
| (1,1895) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HB2 | 17 | 0.22 |
| (1,1895) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HB2 | 17 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1895) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HB2 | 17 | 0.22 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE1 | 10 | 0.22 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE2 | 10 | 0.22 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE3 | 10 | 0.22 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE1 | 15 | 0.22 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE2 | 15 | 0.22 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE3 | 15 | 0.22 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 5 | 0.22 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 18 | 0.22 |
| (1,1785) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD2 | 20 | 0.22 |
| (1,1778) | 1:72:A:THR:HB | 1:73:A:GLN:HB3 | 2 | 0.22 |
| (1,1698) | 1:136:A:GLN:HB2 | 1:136:A:GLN:HG2 | 2 | 0.22 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 10 | 0.22 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 2 | 0.22 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 3 | 0.22 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 4 | 0.22 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 8 | 0.22 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 9 | 0.22 |
| (1,1526) | 1:63:A:PHE:HB2 | 1:64:A:LEU:H | 4 | 0.22 |
| (1,1521) | 1:173:A:PHE:HD1 | 1:177:A:TYR:HB3 | 16 | 0.22 |
| (1,1521) | 1:173:A:PHE:HD2 | 1:177:A:TYR:HB3 | 16 | 0.22 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 4 | 0.22 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 4 | 0.22 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 4 | 0.22 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 14 | 0.22 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 14 | 0.22 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 14 | 0.22 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 20 | 0.22 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 20 | 0.22 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 20 | 0.22 |
| (1,1473) | 1:36:A:PHE:HB2 | 1:40:A:LEU:HD11 | 18 | 0.22 |
| (1,1473) | 1:36:A:PHE:HB2 | 1:40:A:LEU:HD12 | 18 | 0.22 |
| (1,1473) | 1:36:A:PHE:HB2 | 1:40:A:LEU:HD13 | 18 | 0.22 |
| (1,1426) | 1:143:A:ASP:HB2 | 1:144:A:LEU:HG | 3 | 0.22 |
| (1,1366) | 1:34:A:TYR:HE1 | 1:97:A:LYS:HE3 | 2 | 0.22 |
| (1,1366) | 1:34:A:TYR:HE2 | 1:97:A:LYS:HE3 | 2 | 0.22 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG21 | 2 | 0.22 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG22 | 2 | 0.22 |
| (1,1348) | 1:131:A:LYS:HE2 | 1:134:A:VAL:HG23 | 2 | 0.22 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG21 | 2 | 0.22 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG22 | 2 | 0.22 |
| (1,1348) | 1:131:A:LYS:HE3 | 1:134:A:VAL:HG23 | 2 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 2 | 0.22 |
| (1,1331) | 1:70:A:ASP:HB3 | 1:72:A:THR:H | 20 | 0.22 |
| (1,1101) | 1:9:A:TYR:H | 1:10:A:ILE:HG13 | 18 | 0.22 |
| (1,1080) | 1:34:A:TYR:HD1 | 1:38:A:GLU:H | 4 | 0.22 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 8 | 0.22 |
| (1,1005) | 1:46:A:VAL:HG21 | 1:48:A:GLN:H | 18 | 0.22 |
| (1,1005) | 1:46:A:VAL:HG22 | 1:48:A:GLN:H | 18 | 0.22 |
| (1,1005) | 1:46:A:VAL:HG23 | 1:48:A:GLN:H | 18 | 0.22 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 7 | 0.22 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 20 | 0.22 |
| (1,967) | 1:126:A:ASN:HB2 | 1:126:A:ASN:HD22 | 5 | 0.22 |
| (1,967) | 1:126:A:ASN:HB2 | 1:126:A:ASN:HD22 | 12 | 0.22 |
| (1,967) | 1:126:A:ASN:HB2 | 1:126:A:ASN:HD22 | 20 | 0.22 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 16 | 0.22 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 16 | 0.22 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 16 | 0.22 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 4 | 0.22 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 4 | 0.22 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 4 | 0.22 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 15 | 0.22 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 15 | 0.22 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 15 | 0.22 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 17 | 0.22 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 17 | 0.22 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 17 | 0.22 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 3 | 0.22 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 13 | 0.22 |
| (1,650) | 1:145:A:GLN:HA | 1:146:A:LEU:H | 16 | 0.22 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 11 | 0.22 |
| (1,599) | 1:183:A:GLN:HB3 | 1:184:A:LEU:H | 6 | 0.22 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 4 | 0.22 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 4 | 0.22 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 4 | 0.22 |
| (1,587) | 1:46:A:VAL:HG21 | 1:47:A:ARG:H | 9 | 0.22 |
| (1,587) | 1:46:A:VAL:HG22 | 1:47:A:ARG:H | 9 | 0.22 |
| (1,587) | 1:46:A:VAL:HG23 | 1:47:A:ARG:H | 9 | 0.22 |
| (1,577) | 1:121:A:TYR:HB2 | 1:122:A:ASP:H | 9 | 0.22 |
| (1,577) | 1:121:A:TYR:HB2 | 1:122:A:ASP:H | 19 | 0.22 |
| (1,571) | 1:50:A:LEU:H | 1:50:A:LEU:HG | 7 | 0.22 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 2 | 0.22 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 2 | 0.22 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 2 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 8 | 0.22 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 8 | 0.22 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 8 | 0.22 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 10 | 0.22 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 10 | 0.22 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 10 | 0.22 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 14 | 0.22 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 14 | 0.22 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 14 | 0.22 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 20 | 0.22 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 20 | 0.22 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 20 | 0.22 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 6 | 0.22 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 6 | 0.22 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 6 | 0.22 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 15 | 0.22 |
| (1,401) | 1:117:A:LYS:HB2 | 1:120:A:ASP:H | 4 | 0.22 |
| (1,353) | 1:108:A:ARG:HG3 | 1:112:A:VAL:H | 5 | 0.22 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 1 | 0.22 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 1 | 0.22 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 1 | 0.22 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 5 | 0.22 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 5 | 0.22 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 5 | 0.22 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 9 | 0.22 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 9 | 0.22 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 9 | 0.22 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 17 | 0.22 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 17 | 0.22 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 17 | 0.22 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 19 | 0.22 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 19 | 0.22 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 19 | 0.22 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 5 | 0.22 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 5 | 0.22 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 5 | 0.22 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 14 | 0.22 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 14 | 0.22 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 14 | 0.22 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 18 | 0.22 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 18 | 0.22 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 18 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 4 | 0.22 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 4 | 0.22 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 4 | 0.22 |
| (1,165) | 1:67:A:LEU:H | 1:69:A:LYS:H | 3 | 0.22 |
| (1,132) | 1:56:A:MET:HB2 | 1:57:A:THR:H | 15 | 0.22 |
| (1,127) | 1:105:A:ALA:H | 1:107:A:ILE:HB | 14 | 0.22 |
| (1,83) | 1:6:A:GLY:H | 1:11:A:THR:H | 11 | 0.22 |
| (1,67) | 1:26:A:PHE:H | 1:59:A:TYR:H | 1 | 0.22 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 13 | 0.22 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 7 | 0.21 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 7 | 0.21 |
| (1,3461) | 1:75:A:TRP:HB3 | 1:75:A:TRP:HE3 | 14 | 0.21 |
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 14 | 0.21 |
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 14 | 0.21 |
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 18 | 0.21 |
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 18 | 0.21 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 13 | 0.21 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 13 | 0.21 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD1 | 17 | 0.21 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD2 | 17 | 0.21 |
| (1,3231) | 1:88:A:THR:HG21 | 1:90:A:PRO:HD3 | 3 | 0.21 |
| (1,3231) | 1:88:A:THR:HG22 | 1:90:A:PRO:HD3 | 3 | 0.21 |
| (1,3231) | 1:88:A:THR:HG23 | 1:90:A:PRO:HD3 | 3 | 0.21 |
| (1,3230) | 1:87:A:ILE:HA | 1:90:A:PRO:HD3 | 10 | 0.21 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD11 | 19 | 0.21 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD12 | 19 | 0.21 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD13 | 19 | 0.21 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD11 | 19 | 0.21 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD12 | 19 | 0.21 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD13 | 19 | 0.21 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD11 | 19 | 0.21 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD12 | 19 | 0.21 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD13 | 19 | 0.21 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG21 | 13 | 0.21 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG22 | 13 | 0.21 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG23 | 13 | 0.21 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG21 | 13 | 0.21 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG22 | 13 | 0.21 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG23 | 13 | 0.21 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG21 | 13 | 0.21 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG22 | 13 | 0.21 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG23 | 13 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD21 | 19 | 0.21 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD22 | 19 | 0.21 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD23 | 19 | 0.21 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 4 | 0.21 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 7 | 0.21 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 7 | 0.21 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 7 | 0.21 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 11 | 0.21 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 11 | 0.21 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 11 | 0.21 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 18 | 0.21 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 18 | 0.21 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 18 | 0.21 |
| (1,2778) | 1:153:A:TYR:HA | 1:154:A:VAL:HG21 | 14 | 0.21 |
| (1,2778) | 1:153:A:TYR:HA | 1:154:A:VAL:HG22 | 14 | 0.21 |
| (1,2778) | 1:153:A:TYR:HA | 1:154:A:VAL:HG23 | 14 | 0.21 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 7 | 0.21 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 7 | 0.21 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 7 | 0.21 |
| (1,2753) | 1:61:A:VAL:HG11 | 1:62:A:GLU:HA | 11 | 0.21 |
| (1,2753) | 1:61:A:VAL:HG12 | 1:62:A:GLU:HA | 11 | 0.21 |
| (1,2753) | 1:61:A:VAL:HG13 | 1:62:A:GLU:HA | 11 | 0.21 |
| (1,2753) | 1:61:A:VAL:HG11 | 1:62:A:GLU:HA | 14 | 0.21 |
| (1,2753) | 1:61:A:VAL:HG12 | 1:62:A:GLU:HA | 14 | 0.21 |
| (1,2753) | 1:61:A:VAL:HG13 | 1:62:A:GLU:HA | 14 | 0.21 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 6 | 0.21 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 6 | 0.21 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 6 | 0.21 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 18 | 0.21 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 18 | 0.21 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 18 | 0.21 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG21 | 6 | 0.21 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG22 | 6 | 0.21 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG23 | 6 | 0.21 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG21 | 6 | 0.21 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG22 | 6 | 0.21 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG23 | 6 | 0.21 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG21 | 6 | 0.21 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG22 | 6 | 0.21 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG23 | 6 | 0.21 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 1 | 0.21 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 1 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 1 | 0.21 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 12 | 0.21 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 12 | 0.21 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 12 | 0.21 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 12 | 0.21 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 12 | 0.21 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 12 | 0.21 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 12 | 0.21 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 12 | 0.21 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 12 | 0.21 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG21 | 5 | 0.21 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG22 | 5 | 0.21 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG23 | 5 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG21 | 16 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG22 | 16 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG23 | 16 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG21 | 16 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG22 | 16 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG23 | 16 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG21 | 16 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG22 | 16 | 0.21 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG23 | 16 | 0.21 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 1 | 0.21 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE1 | 13 | 0.21 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE2 | 13 | 0.21 |
| (1,2436) | 1:46:A:VAL:HG11 | 1:56:A:MET:HE3 | 13 | 0.21 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE1 | 13 | 0.21 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE2 | 13 | 0.21 |
| (1,2436) | 1:46:A:VAL:HG12 | 1:56:A:MET:HE3 | 13 | 0.21 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE1 | 13 | 0.21 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE2 | 13 | 0.21 |
| (1,2436) | 1:46:A:VAL:HG13 | 1:56:A:MET:HE3 | 13 | 0.21 |
| (1,2339) | 1:186:A:GLU:HG3 | 1:187:A:LYS:HG2 | 8 | 0.21 |
| (1,2315) | 1:46:A:VAL:HG21 | 1:50:A:LEU:HG | 20 | 0.21 |
| (1,2315) | 1:46:A:VAL:HG22 | 1:50:A:LEU:HG | 20 | 0.21 |
| (1,2315) | 1:46:A:VAL:HG23 | 1:50:A:LEU:HG | 20 | 0.21 |
| (1,2274) | 1:4:A:THR:HA | 1:7:A:LYS:HB2 | 20 | 0.21 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 10 | 0.21 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 10 | 0.21 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 10 | 0.21 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 10 | 0.21 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 10 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 10 | 0.21 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 4 | 0.21 |
| (1,2159) | 1:76:A:ALA:HA | 1:79:A:ILE:HG12 | 1 | 0.21 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 11 | 0.21 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 11 | 0.21 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 11 | 0.21 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB2 | 19 | 0.21 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB3 | 19 | 0.21 |
| (1,2072) | 1:93:A:GLU:HA | 1:97:A:LYS:HD2 | 3 | 0.21 |
| (1,2025) | 1:69:A:LYS:H | 1:69:A:LYS:HD3 | 18 | 0.21 |
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 19 | 0.21 |
| (1,1981) | 1:187:A:LYS:H | 1:187:A:LYS:HD3 | 3 | 0.21 |
| (1,1981) | 1:187:A:LYS:H | 1:187:A:LYS:HD3 | 13 | 0.21 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 8 | 0.21 |
| (1,1931) | 1:62:A:GLU:HB2 | 1:63:A:PHE:HB3 | 13 | 0.21 |
| (1,1931) | 1:62:A:GLU:HB3 | 1:63:A:PHE:HB3 | 13 | 0.21 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG21 | 12 | 0.21 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG22 | 12 | 0.21 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG23 | 12 | 0.21 |
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 17 | 0.21 |
| (1,1792) | 1:56:A:MET:HB2 | 1:56:A:MET:HG3 | 7 | 0.21 |
| (1,1703) | 1:59:A:TYR:HE1 | 1:136:A:GLN:HG3 | 16 | 0.21 |
| (1,1703) | 1:59:A:TYR:HE2 | 1:136:A:GLN:HG3 | 16 | 0.21 |
| (1,1699) | 1:135:A:ALA:HB1 | 1:136:A:GLN:HG2 | 20 | 0.21 |
| (1,1699) | 1:135:A:ALA:HB2 | 1:136:A:GLN:HG2 | 20 | 0.21 |
| (1,1699) | 1:135:A:ALA:HB3 | 1:136:A:GLN:HG2 | 20 | 0.21 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 15 | 0.21 |
| (1,1695) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HE22 | 8 | 0.21 |
| (1,1685) | 1:99:A:GLN:HA | 1:99:A:GLN:HG3 | 11 | 0.21 |
| (1,1624) | 1:33:A:CYS:HA | 1:150:A:PRO:HB2 | 10 | 0.21 |
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 18 | 0.21 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 18 | 0.21 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 18 | 0.21 |
| (1,1513) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB2 | 9 | 0.21 |
| (1,1513) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB2 | 9 | 0.21 |
| (1,1513) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB2 | 9 | 0.21 |
| (1,1513) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB2 | 20 | 0.21 |
| (1,1513) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB2 | 20 | 0.21 |
| (1,1513) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB2 | 20 | 0.21 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 6 | 0.21 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 6 | 0.21 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 6 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1470) | 1:173:A:PHE:HB3 | 1:174:A:VAL:HG11 | 2 | 0.21 |
| (1,1470) | 1:173:A:PHE:HB3 | 1:174:A:VAL:HG12 | 2 | 0.21 |
| (1,1470) | 1:173:A:PHE:HB3 | 1:174:A:VAL:HG13 | 2 | 0.21 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 11 | 0.21 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 11 | 0.21 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 11 | 0.21 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB2 | 15 | 0.21 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB3 | 15 | 0.21 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB2 | 17 | 0.21 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB3 | 17 | 0.21 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE2 | 20 | 0.21 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE3 | 20 | 0.21 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE2 | 20 | 0.21 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE3 | 20 | 0.21 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE2 | 20 | 0.21 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE3 | 20 | 0.21 |
| (1,1343) | 1:181:A:VAL:HA | 1:184:A:LEU:HB3 | 7 | 0.21 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 20 | 0.21 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 20 | 0.21 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 20 | 0.21 |
| (1,1331) | 1:70:A:ASP:HB3 | 1:72:A:THR:H | 15 | 0.21 |
| (1,1215) | 1:73:A:GLN:HE21 | 1:77:A:VAL:HG21 | 11 | 0.21 |
| (1,1215) | 1:73:A:GLN:HE21 | 1:77:A:VAL:HG22 | 11 | 0.21 |
| (1,1215) | 1:73:A:GLN:HE21 | 1:77:A:VAL:HG23 | 11 | 0.21 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG11 | 7 | 0.21 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG12 | 7 | 0.21 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG13 | 7 | 0.21 |
| (1,1080) | 1:34:A:TYR:HD1 | 1:38:A:GLU:H | 7 | 0.21 |
| (1,1080) | 1:34:A:TYR:HD1 | 1:38:A:GLU:H | 17 | 0.21 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 14 | 0.21 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG21 | 2 | 0.21 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG22 | 2 | 0.21 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG23 | 2 | 0.21 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG21 | 16 | 0.21 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG22 | 16 | 0.21 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG23 | 16 | 0.21 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 4 | 0.21 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 14 | 0.21 |
| (1,967) | 1:126:A:ASN:HB2 | 1:126:A:ASN:HD22 | 4 | 0.21 |
| (1,967) | 1:126:A:ASN:HB2 | 1:126:A:ASN:HD22 | 10 | 0.21 |
| (1,967) | 1:126:A:ASN:HB2 | 1:126:A:ASN:HD22 | 15 | 0.21 |
| (1,967) | 1:126:A:ASN:HB2 | 1:126:A:ASN:HD22 | 18 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,967) | 1:126:A:ASN:HB2 | 1:126:A:ASN:HD22 | 19 | 0.21 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 14 | 0.21 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 20 | 0.21 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 13 | 0.21 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 13 | 0.21 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 13 | 0.21 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 19 | 0.21 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 19 | 0.21 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 19 | 0.21 |
| (1,815) | 1:91:A:MET:HB2 | 1:93:A:GLU:H | 1 | 0.21 |
| (1,678) | 1:71:A:LEU:HD21 | 1:72:A:THR:H | 14 | 0.21 |
| (1,678) | 1:71:A:LEU:HD22 | 1:72:A:THR:H | 14 | 0.21 |
| (1,678) | 1:71:A:LEU:HD23 | 1:72:A:THR:H | 14 | 0.21 |
| (1,650) | 1:145:A:GLN:HA | 1:146:A:LEU:H | 2 | 0.21 |
| (1,650) | 1:145:A:GLN:HA | 1:146:A:LEU:H | 17 | 0.21 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 12 | 0.21 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 12 | 0.21 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 12 | 0.21 |
| (1,568) | 1:49:A:LYS:HA | 1:50:A:LEU:H | 10 | 0.21 |
| (1,560) | 1:42:A:VAL:HG21 | 1:178:A:ALA:H | 1 | 0.21 |
| (1,560) | 1:42:A:VAL:HG22 | 1:178:A:ALA:H | 1 | 0.21 |
| (1,560) | 1:42:A:VAL:HG23 | 1:178:A:ALA:H | 1 | 0.21 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 6 | 0.21 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 6 | 0.21 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 6 | 0.21 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 15 | 0.21 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 15 | 0.21 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 15 | 0.21 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 11 | 0.21 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 11 | 0.21 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 11 | 0.21 |
| (1,380) | 1:138:A:GLU:H | 1:138:A:GLU:HG3 | 15 | 0.21 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 3 | 0.21 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 3 | 0.21 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 3 | 0.21 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 8 | 0.21 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 8 | 0.21 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 8 | 0.21 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 13 | 0.21 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 13 | 0.21 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 13 | 0.21 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 15 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 15 | 0.21 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 15 | 0.21 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 12 | 0.21 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 12 | 0.21 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 12 | 0.21 |
| (1,300) | 1:130:A:VAL:HG21 | 1:131:A:LYS:H | 17 | 0.21 |
| (1,300) | 1:130:A:VAL:HG22 | 1:131:A:LYS:H | 17 | 0.21 |
| (1,300) | 1:130:A:VAL:HG23 | 1:131:A:LYS:H | 17 | 0.21 |
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 7 | 0.21 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 12 | 0.21 |
| (1,241) | 1:70:A:ASP:HB2 | 1:74:A:ALA:H | 14 | 0.21 |
| (1,184) | 1:60:A:HIS:H | 1:72:A:THR:HA | 7 | 0.21 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD21 | 9 | 0.21 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD22 | 9 | 0.21 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD23 | 9 | 0.21 |
| (1,67) | 1:26:A:PHE:H | 1:59:A:TYR:H | 4 | 0.21 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB2 | 13 | 0.2 |
| (1,3504) | 1:158:A:TYR:HE1 | 1:187:A:LYS:HB3 | 13 | 0.2 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB2 | 13 | 0.2 |
| (1,3504) | 1:158:A:TYR:HE2 | 1:187:A:LYS:HB3 | 13 | 0.2 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 3 | 0.2 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 3 | 0.2 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 13 | 0.2 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 13 | 0.2 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 18 | 0.2 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 18 | 0.2 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 10 | 0.2 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 13 | 0.2 |
| (1,3420) | 1:60:A:HIS:HB3 | 1:75:A:TRP:HD1 | 6 | 0.2 |
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 1 | 0.2 |
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 1 | 0.2 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD1 | 4 | 0.2 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD2 | 4 | 0.2 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD1 | 11 | 0.2 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD2 | 11 | 0.2 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 13 | 0.2 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 13 | 0.2 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 13 | 0.2 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 13 | 0.2 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 13 | 0.2 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 13 | 0.2 |
| (1,3277) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA3 | 2 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3277) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA3 | 2 | 0.2 |
| (1,3277) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA3 | 2 | 0.2 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE1 | 14 | 0.2 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE2 | 14 | 0.2 |
| (1,3135) | 1:42:A:VAL:HG21 | 1:152:A:MET:HE3 | 14 | 0.2 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE1 | 14 | 0.2 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE2 | 14 | 0.2 |
| (1,3135) | 1:42:A:VAL:HG22 | 1:152:A:MET:HE3 | 14 | 0.2 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE1 | 14 | 0.2 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE2 | 14 | 0.2 |
| (1,3135) | 1:42:A:VAL:HG23 | 1:152:A:MET:HE3 | 14 | 0.2 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 20 | 0.2 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 20 | 0.2 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 20 | 0.2 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 20 | 0.2 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 20 | 0.2 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 20 | 0.2 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG21 | 11 | 0.2 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG22 | 11 | 0.2 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG23 | 11 | 0.2 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG21 | 11 | 0.2 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG22 | 11 | 0.2 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG23 | 11 | 0.2 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG21 | 11 | 0.2 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG22 | 11 | 0.2 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG23 | 11 | 0.2 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE1 | 10 | 0.2 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE2 | 10 | 0.2 |
| (1,3067) | 1:46:A:VAL:HA | 1:56:A:MET:HE3 | 10 | 0.2 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD21 | 7 | 0.2 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD22 | 7 | 0.2 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD23 | 7 | 0.2 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 4 | 0.2 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 4 | 0.2 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 4 | 0.2 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 1 | 0.2 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 1 | 0.2 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 1 | 0.2 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 15 | 0.2 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 15 | 0.2 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 15 | 0.2 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 17 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2753) | 1:61:A:VAL:HG11 | 1:62:A:GLU:HA | 17 | 0.2 |
| (1,2753) | 1:61:A:VAL:HG12 | 1:62:A:GLU:HA | 17 | 0.2 |
| (1,2753) | 1:61:A:VAL:HG13 | 1:62:A:GLU:HA | 17 | 0.2 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 17 | 0.2 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 17 | 0.2 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 17 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG21 | 2 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG22 | 2 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG23 | 2 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG21 | 2 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG22 | 2 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG23 | 2 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG21 | 2 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG22 | 2 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG23 | 2 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG21 | 16 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG22 | 16 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG23 | 16 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG21 | 16 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG22 | 16 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG23 | 16 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG21 | 16 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG22 | 16 | 0.2 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG23 | 16 | 0.2 |
| (1,2622) | 1:149:A:VAL:HA | 1:151:A:ALA:H | 1 | 0.2 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 15 | 0.2 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 15 | 0.2 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 15 | 0.2 |
| (1,2588) | 1:70:A:ASP:HA | 1:72:A:THR:H | 18 | 0.2 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 19 | 0.2 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 19 | 0.2 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 19 | 0.2 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD21 | 11 | 0.2 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD22 | 11 | 0.2 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD23 | 11 | 0.2 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD21 | 16 | 0.2 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD22 | 16 | 0.2 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD23 | 16 | 0.2 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 12 | 0.2 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 6 | 0.2 |
| (1,2315) | 1:46:A:VAL:HG21 | 1:50:A:LEU:HG | 4 | 0.2 |
| (1,2315) | 1:46:A:VAL:HG22 | 1:50:A:LEU:HG | 4 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2315) | 1:46:A:VAL:HG23 | 1:50:A:LEU:HG | 4 | 0.2 |
| (1,2195) | 1:66:A:PRO:HD2 | 1:67:A:LEU:HG | 14 | 0.2 |
| (1,2159) | 1:76:A:ALA:HA | 1:79:A:ILE:HG12 | 16 | 0.2 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 1 | 0.2 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 1 | 0.2 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 1 | 0.2 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG21 | 10 | 0.2 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG22 | 10 | 0.2 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG23 | 10 | 0.2 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG21 | 10 | 0.2 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG22 | 10 | 0.2 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG23 | 10 | 0.2 |
| (1,2072) | 1:93:A:GLU:HA | 1:97:A:LYS:HD2 | 4 | 0.2 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 6 | 0.2 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 12 | 0.2 |
| (1,2015) | 1:117:A:LYS:HB2 | 1:117:A:LYS:HD3 | 7 | 0.2 |
| (1,1981) | 1:187:A:LYS:H | 1:187:A:LYS:HD3 | 14 | 0.2 |
| (1,1915) | 1:186:A:GLU:HB2 | 1:187:A:LYS:H | 9 | 0.2 |
| (1,1915) | 1:186:A:GLU:HB2 | 1:187:A:LYS:H | 16 | 0.2 |
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 13 | 0.2 |
| (1,1873) | 1:46:A:VAL:HA | 1:49:A:LYS:HB3 | 17 | 0.2 |
| (1,1832) | 1:124:A:ALA:HB1 | 1:130:A:VAL:HB | 16 | 0.2 |
| (1,1832) | 1:124:A:ALA:HB2 | 1:130:A:VAL:HB | 16 | 0.2 |
| (1,1832) | 1:124:A:ALA:HB3 | 1:130:A:VAL:HB | 16 | 0.2 |
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 3 | 0.2 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 9 | 0.2 |
| (1,1792) | 1:56:A:MET:HB2 | 1:56:A:MET:HG3 | 6 | 0.2 |
| (1,1785) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD2 | 3 | 0.2 |
| (1,1758) | 1:14:A:LYS:H | 1:14:A:LYS:HB3 | 14 | 0.2 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 1 | 0.2 |
| (1,1744) | 1:134:A:VAL:HA | 1:137:A:GLN:HG2 | 16 | 0.2 |
| (1,1744) | 1:134:A:VAL:HA | 1:137:A:GLN:HG2 | 17 | 0.2 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 11 | 0.2 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 20 | 0.2 |
| (1,1695) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HE22 | 13 | 0.2 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG2 | 14 | 0.2 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG3 | 14 | 0.2 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG2 | 17 | 0.2 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG3 | 17 | 0.2 |
| (1,1685) | 1:99:A:GLN:HA | 1:99:A:GLN:HG3 | 18 | 0.2 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 1 | 0.2 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 13 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1565) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 4 | 0.2 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB2 | 18 | 0.2 |
| (1,1534) | 1:34:A:TYR:HB2 | 1:35:A:GLN:HB3 | 18 | 0.2 |
| (1,1526) | 1:63:A:PHE:HB2 | 1:64:A:LEU:H | 3 | 0.2 |
| (1,1513) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB2 | 15 | 0.2 |
| (1,1513) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB2 | 15 | 0.2 |
| (1,1513) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB2 | 15 | 0.2 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 16 | 0.2 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 16 | 0.2 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 16 | 0.2 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 15 | 0.2 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG11 | 12 | 0.2 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG12 | 12 | 0.2 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG13 | 12 | 0.2 |
| (1,1438) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HB2 | 8 | 0.2 |
| (1,1438) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HB2 | 8 | 0.2 |
| (1,1438) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HB2 | 8 | 0.2 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG21 | 12 | 0.2 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG22 | 12 | 0.2 |
| (1,1405) | 1:166:A:ASP:HB3 | 1:172:A:VAL:HG23 | 12 | 0.2 |
| (1,1366) | 1:34:A:TYR:HE1 | 1:97:A:LYS:HE3 | 20 | 0.2 |
| (1,1366) | 1:34:A:TYR:HE2 | 1:97:A:LYS:HE3 | 20 | 0.2 |
| (1,1265) | 1:64:A:LEU:HB3 | 1:65:A:GLY:HA2 | 14 | 0.2 |
| (1,1262) | 1:29:A:TYR:HB3 | 1:64:A:LEU:HB2 | 2 | 0.2 |
| (1,1059) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HG3 | 1 | 0.2 |
| (1,1059) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HG3 | 14 | 0.2 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 2 | 0.2 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 8 | 0.2 |
| (1,883) | 1:49:A:LYS:H | 1:49:A:LYS:HD3 | 8 | 0.2 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 6 | 0.2 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 6 | 0.2 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 6 | 0.2 |
| (1,650) | 1:145:A:GLN:HA | 1:146:A:LEU:H | 15 | 0.2 |
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 6 | 0.2 |
| (1,560) | 1:42:A:VAL:HG21 | 1:178:A:ALA:H | 5 | 0.2 |
| (1,560) | 1:42:A:VAL:HG22 | 1:178:A:ALA:H | 5 | 0.2 |
| (1,560) | 1:42:A:VAL:HG23 | 1:178:A:ALA:H | 5 | 0.2 |
| (1,555) | 1:174:A:VAL:HG21 | 1:178:A:ALA:H | 15 | 0.2 |
| (1,555) | 1:174:A:VAL:HG22 | 1:178:A:ALA:H | 15 | 0.2 |
| (1,555) | 1:174:A:VAL:HG23 | 1:178:A:ALA:H | 15 | 0.2 |
| (1,555) | 1:174:A:VAL:HG21 | 1:178:A:ALA:H | 20 | 0.2 |
| (1,555) | 1:174:A:VAL:HG22 | 1:178:A:ALA:H | 20 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,555) | 1:174:A:VAL:HG23 | 1:178:A:ALA:H | 20 | 0.2 |
| (1,485) | 1:4:A:THR:H | 1:7:A:LYS:HB2 | 2 | 0.2 |
| (1,441) | 1:34:A:TYR:HE1 | 1:92:A:PHE:H | 11 | 0.2 |
| (1,401) | 1:117:A:LYS:HB2 | 1:120:A:ASP:H | 3 | 0.2 |
| (1,337) | 1:166:A:ASP:H | 1:176:A:GLN:HE21 | 6 | 0.2 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 6 | 0.2 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 6 | 0.2 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 6 | 0.2 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 3 | 0.2 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 7 | 0.2 |
| (1,216) | 1:34:A:TYR:H | 1:96:A:GLN:HE21 | 1 | 0.2 |
| (1,216) | 1:34:A:TYR:H | 1:96:A:GLN:HE21 | 12 | 0.2 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD21 | 18 | 0.2 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD22 | 18 | 0.2 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD23 | 18 | 0.2 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 4 | 0.2 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 7 | 0.19 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 7 | 0.19 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 7 | 0.19 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 7 | 0.19 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 7 | 0.19 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 7 | 0.19 |
| (1,3495) | 1:23:A:LEU:HD21 | 1:59:A:TYR:HE1 | 4 | 0.19 |
| (1,3495) | 1:23:A:LEU:HD21 | 1:59:A:TYR:HE2 | 4 | 0.19 |
| (1,3495) | 1:23:A:LEU:HD22 | 1:59:A:TYR:HE1 | 4 | 0.19 |
| (1,3495) | 1:23:A:LEU:HD22 | 1:59:A:TYR:HE2 | 4 | 0.19 |
| (1,3495) | 1:23:A:LEU:HD23 | 1:59:A:TYR:HE1 | 4 | 0.19 |
| (1,3495) | 1:23:A:LEU:HD23 | 1:59:A:TYR:HE2 | 4 | 0.19 |
| (1,3481) | 1:29:A:TYR:HE1 | 1:67:A:LEU:HA | 5 | 0.19 |
| (1,3481) | 1:29:A:TYR:HE2 | 1:67:A:LEU:HA | 5 | 0.19 |
| (1,3461) | 1:75:A:TRP:HB3 | 1:75:A:TRP:HE3 | 10 | 0.19 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 17 | 0.19 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG2 | 4 | 0.19 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG3 | 4 | 0.19 |
| (1,3419) | 1:75:A:TRP:HB2 | 1:75:A:TRP:HD1 | 6 | 0.19 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD11 | 14 | 0.19 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD12 | 14 | 0.19 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD13 | 14 | 0.19 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD11 | 14 | 0.19 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD12 | 14 | 0.19 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD13 | 14 | 0.19 |
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD1 | 8 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3309) | 1:154:A:VAL:HG21 | 1:158:A:TYR:HD2 | 8 | 0.19 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD1 | 8 | 0.19 |
| (1,3309) | 1:154:A:VAL:HG22 | 1:158:A:TYR:HD2 | 8 | 0.19 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD1 | 8 | 0.19 |
| (1,3309) | 1:154:A:VAL:HG23 | 1:158:A:TYR:HD2 | 8 | 0.19 |
| (1,3230) | 1:87:A:ILE:HA | 1:90:A:PRO:HD3 | 13 | 0.19 |
| (1,3229) | 1:88:A:THR:H | 1:90:A:PRO:HD3 | 6 | 0.19 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 11 | 0.19 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 11 | 0.19 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 11 | 0.19 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 11 | 0.19 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 11 | 0.19 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 11 | 0.19 |
| (1,3112) | 1:67:A:LEU:HA | 1:70:A:ASP:HB3 | 3 | 0.19 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG21 | 12 | 0.19 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG22 | 12 | 0.19 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG23 | 12 | 0.19 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG21 | 12 | 0.19 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG22 | 12 | 0.19 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG23 | 12 | 0.19 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG21 | 12 | 0.19 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG22 | 12 | 0.19 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG23 | 12 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 6 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 6 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 6 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 6 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 6 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 6 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 6 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 6 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 6 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 7 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 7 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 7 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 7 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 7 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 7 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 7 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 7 | 0.19 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 7 | 0.19 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG11 | 4 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG12 | 4 | 0.19 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG13 | 4 | 0.19 |
| (1,2935) | 1:75:A:TRP:HA | 1:78:A:ALA:HA | 3 | 0.19 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 2 | 0.19 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 2 | 0.19 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 2 | 0.19 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 3 | 0.19 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 3 | 0.19 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 3 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG11 | 1 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG12 | 1 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG13 | 1 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG11 | 1 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG12 | 1 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG13 | 1 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG11 | 1 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG12 | 1 | 0.19 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG13 | 1 | 0.19 |
| (1,2908) | 1:175:A:ALA:HA | 1:178:A:ALA:H | 12 | 0.19 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 12 | 0.19 |
| (1,2766) | 1:39:A:VAL:HG21 | 1:40:A:LEU:H | 14 | 0.19 |
| (1,2766) | 1:39:A:VAL:HG22 | 1:40:A:LEU:H | 14 | 0.19 |
| (1,2766) | 1:39:A:VAL:HG23 | 1:40:A:LEU:H | 14 | 0.19 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 16 | 0.19 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 16 | 0.19 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 16 | 0.19 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 5 | 0.19 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 5 | 0.19 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 5 | 0.19 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 12 | 0.19 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 12 | 0.19 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 12 | 0.19 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 19 | 0.19 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 19 | 0.19 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 19 | 0.19 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG21 | 1 | 0.19 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG22 | 1 | 0.19 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG23 | 1 | 0.19 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG21 | 1 | 0.19 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG22 | 1 | 0.19 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG23 | 1 | 0.19 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG21 | 1 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG22 | 1 | 0.19 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG23 | 1 | 0.19 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 16 | 0.19 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 16 | 0.19 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 16 | 0.19 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD21 | 14 | 0.19 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD22 | 14 | 0.19 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD23 | 14 | 0.19 |
| (1,2392) | 1:31:A:PRO:HA | 1:34:A:TYR:HA | 19 | 0.19 |
| (1,2347) | 1:131:A:LYS:HG3 | 1:131:A:LYS:HD2 | 2 | 0.19 |
| (1,2347) | 1:131:A:LYS:HG3 | 1:131:A:LYS:HD2 | 14 | 0.19 |
| (1,2279) | 1:73:A:GLN:HG3 | 1:125:A:TRP:HA | 16 | 0.19 |
| (1,2279) | 1:73:A:GLN:HG3 | 1:125:A:TRP:HA | 18 | 0.19 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 17 | 0.19 |
| (1,2214) | 1:120:A:ASP:HB2 | 1:121:A:TYR:HA | 18 | 0.19 |
| (1,2177) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HG3 | 11 | 0.19 |
| (1,2177) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HG3 | 11 | 0.19 |
| (1,2156) | 1:35:A:GLN:HG2 | 1:40:A:LEU:HG | 7 | 0.19 |
| (1,2156) | 1:35:A:GLN:HG3 | 1:40:A:LEU:HG | 7 | 0.19 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 11 | 0.19 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 11 | 0.19 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 12 | 0.19 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 12 | 0.19 |
| (1,2118) | 1:10:A:ILE:HG13 | 1:159:A:GLN:H | 17 | 0.19 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 2 | 0.19 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 20 | 0.19 |
| (1,1930) | 1:186:A:GLU:HB3 | 1:187:A:LYS:H | 7 | 0.19 |
| (1,1848) | 1:83:A:VAL:HB | 1:87:A:ILE:HG13 | 15 | 0.19 |
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 19 | 0.19 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD1 | 2 | 0.19 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD2 | 2 | 0.19 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 20 | 0.19 |
| (1,1785) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD2 | 11 | 0.19 |
| (1,1758) | 1:14:A:LYS:H | 1:14:A:LYS:HB3 | 4 | 0.19 |
| (1,1738) | 1:101:A:VAL:HG11 | 1:102:A:GLN:HG3 | 3 | 0.19 |
| (1,1738) | 1:101:A:VAL:HG12 | 1:102:A:GLN:HG3 | 3 | 0.19 |
| (1,1738) | 1:101:A:VAL:HG13 | 1:102:A:GLN:HG3 | 3 | 0.19 |
| (1,1730) | 1:55:A:LYS:H | 1:55:A:LYS:HB3 | 18 | 0.19 |
| (1,1730) | 1:55:A:LYS:H | 1:55:A:LYS:HB3 | 19 | 0.19 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 7 | 0.19 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 12 | 0.19 |
| (1,1685) | 1:99:A:GLN:HA | 1:99:A:GLN:HG3 | 8 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1685) | 1:99:A:GLN:HA | 1:99:A:GLN:HG3 | 14 | 0.19 |
| (1,1669) | 1:135:A:ALA:HB1 | 1:138:A:GLU:HG2 | 20 | 0.19 |
| (1,1669) | 1:135:A:ALA:HB2 | 1:138:A:GLU:HG2 | 20 | 0.19 |
| (1,1669) | 1:135:A:ALA:HB3 | 1:138:A:GLU:HG2 | 20 | 0.19 |
| (1,1604) | 1:61:A:VAL:HA | 1:62:A:GLU:HG2 | 19 | 0.19 |
| (1,1603) | 1:62:A:GLU:HG2 | 1:63:A:PHE:H | 11 | 0.19 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG11 | 1 | 0.19 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG12 | 1 | 0.19 |
| (1,1564) | 1:152:A:MET:HB3 | 1:181:A:VAL:HG13 | 1 | 0.19 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD11 | 1 | 0.19 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD12 | 1 | 0.19 |
| (1,1555) | 1:152:A:MET:HB2 | 1:160:A:LEU:HD13 | 1 | 0.19 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG11 | 13 | 0.19 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG12 | 13 | 0.19 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG13 | 13 | 0.19 |
| (1,1474) | 1:161:A:ASN:HB2 | 1:161:A:ASN:HD22 | 7 | 0.19 |
| (1,1438) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HB2 | 10 | 0.19 |
| (1,1438) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HB2 | 10 | 0.19 |
| (1,1438) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HB2 | 10 | 0.19 |
| (1,1438) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HB2 | 17 | 0.19 |
| (1,1438) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HB2 | 17 | 0.19 |
| (1,1438) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HB2 | 17 | 0.19 |
| (1,1427) | 1:143:A:ASP:HB2 | 1:145:A:GLN:HE22 | 20 | 0.19 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 19 | 0.19 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 19 | 0.19 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 19 | 0.19 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB2 | 11 | 0.19 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB3 | 11 | 0.19 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB2 | 13 | 0.19 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB3 | 13 | 0.19 |
| (1,1366) | 1:34:A:TYR:HE1 | 1:97:A:LYS:HE3 | 11 | 0.19 |
| (1,1366) | 1:34:A:TYR:HE2 | 1:97:A:LYS:HE3 | 11 | 0.19 |
| (1,1331) | 1:70:A:ASP:HB3 | 1:72:A:THR:H | 14 | 0.19 |
| (1,1298) | 1:141:A:ALA:HA | 1:146:A:LEU:HB2 | 16 | 0.19 |
| (1,1294) | 1:71:A:LEU:HB2 | 1:74:A:ALA:H | 8 | 0.19 |
| (1,1215) | 1:73:A:GLN:HE21 | 1:77:A:VAL:HG21 | 18 | 0.19 |
| (1,1215) | 1:73:A:GLN:HE21 | 1:77:A:VAL:HG22 | 18 | 0.19 |
| (1,1215) | 1:73:A:GLN:HE21 | 1:77:A:VAL:HG23 | 18 | 0.19 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG11 | 2 | 0.19 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG12 | 2 | 0.19 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG13 | 2 | 0.19 |
| (1,1058) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HA | 6 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 16 | 0.19 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 7 | 0.19 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG21 | 18 | 0.19 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG22 | 18 | 0.19 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG23 | 18 | 0.19 |
| (1,967) | 1:126:A:ASN:HB2 | 1:126:A:ASN:HD22 | 11 | 0.19 |
| (1,967) | 1:126:A:ASN:HB2 | 1:126:A:ASN:HD22 | 17 | 0.19 |
| (1,938) | 1:112:A:VAL:HG11 | 1:118:A:GLY:H | 12 | 0.19 |
| (1,938) | 1:112:A:VAL:HG12 | 1:118:A:GLY:H | 12 | 0.19 |
| (1,938) | 1:112:A:VAL:HG13 | 1:118:A:GLY:H | 12 | 0.19 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 5 | 0.19 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 5 | 0.19 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 5 | 0.19 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 9 | 0.19 |
| (1,886) | 1:46:A:VAL:HG21 | 1:49:A:LYS:H | 7 | 0.19 |
| (1,886) | 1:46:A:VAL:HG22 | 1:49:A:LYS:H | 7 | 0.19 |
| (1,886) | 1:46:A:VAL:HG23 | 1:49:A:LYS:H | 7 | 0.19 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 17 | 0.19 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 17 | 0.19 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 17 | 0.19 |
| (1,815) | 1:91:A:MET:HB2 | 1:93:A:GLU:H | 11 | 0.19 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 1 | 0.19 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 16 | 0.19 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 8 | 0.19 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 6 | 0.19 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 6 | 0.19 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 6 | 0.19 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 14 | 0.19 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 14 | 0.19 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 14 | 0.19 |
| (1,587) | 1:46:A:VAL:HG21 | 1:47:A:ARG:H | 18 | 0.19 |
| (1,587) | 1:46:A:VAL:HG22 | 1:47:A:ARG:H | 18 | 0.19 |
| (1,587) | 1:46:A:VAL:HG23 | 1:47:A:ARG:H | 18 | 0.19 |
| (1,577) | 1:121:A:TYR:HB2 | 1:122:A:ASP:H | 18 | 0.19 |
| (1,568) | 1:49:A:LYS:HA | 1:50:A:LEU:H | 17 | 0.19 |
| (1,568) | 1:49:A:LYS:HA | 1:50:A:LEU:H | 20 | 0.19 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG11 | 12 | 0.19 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG12 | 12 | 0.19 |
| (1,531) | 1:129:A:VAL:H | 1:129:A:VAL:HG13 | 12 | 0.19 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 15 | 0.19 |
| (1,498) | 1:77:A:VAL:HG11 | 1:124:A:ALA:H | 3 | 0.19 |
| (1,498) | 1:77:A:VAL:HG12 | 1:124:A:ALA:H | 3 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,498) | 1:77:A:VAL:HG13 | 1:124:A:ALA:H | 3 | 0.19 |
| (1,485) | 1:4:A:THR:H | 1:7:A:LYS:HB2 | 11 | 0.19 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 1 | 0.19 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 12 | 0.19 |
| (1,380) | 1:138:A:GLU:H | 1:138:A:GLU:HG3 | 2 | 0.19 |
| (1,353) | 1:108:A:ARG:HG3 | 1:112:A:VAL:H | 10 | 0.19 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 20 | 0.19 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 20 | 0.19 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 20 | 0.19 |
| (1,300) | 1:130:A:VAL:HG21 | 1:131:A:LYS:H | 10 | 0.19 |
| (1,300) | 1:130:A:VAL:HG22 | 1:131:A:LYS:H | 10 | 0.19 |
| (1,300) | 1:130:A:VAL:HG23 | 1:131:A:LYS:H | 10 | 0.19 |
| (1,294) | 1:7:A:LYS:H | 1:7:A:LYS:HG3 | 3 | 0.19 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 2 | 0.19 |
| (1,127) | 1:105:A:ALA:H | 1:107:A:ILE:HB | 15 | 0.19 |
| (1,118) | 1:159:A:GLN:H | 1:184:A:LEU:HD21 | 15 | 0.19 |
| (1,118) | 1:159:A:GLN:H | 1:184:A:LEU:HD22 | 15 | 0.19 |
| (1,118) | 1:159:A:GLN:H | 1:184:A:LEU:HD23 | 15 | 0.19 |
| (1,90) | 1:185:A:VAL:HA | 1:188:A:LYS:H | 14 | 0.19 |
| (1,67) | 1:26:A:PHE:H | 1:59:A:TYR:H | 2 | 0.19 |
| (1,40) | 1:5:A:ASP:H | 1:7:A:LYS:HB2 | 11 | 0.19 |
| (1,40) | 1:5:A:ASP:H | 1:7:A:LYS:HB2 | 20 | 0.19 |
| (1,3) | 1:152:A:MET:HB3 | 1:160:A:LEU:H | 2 | 0.19 |
| (1,3523) | 1:73:A:GLN:HE21 | 1:125:A:TRP:HZ2 | 17 | 0.18 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 7 | 0.18 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 7 | 0.18 |
| (1,3486) | 1:29:A:TYR:HE1 | 1:65:A:GLY:HA2 | 8 | 0.18 |
| (1,3486) | 1:29:A:TYR:HE2 | 1:65:A:GLY:HA2 | 8 | 0.18 |
| (1,3485) | 1:29:A:TYR:HE1 | 1:66:A:PRO:HD2 | 6 | 0.18 |
| (1,3485) | 1:29:A:TYR:HE2 | 1:66:A:PRO:HD2 | 6 | 0.18 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 6 | 0.18 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 6 | 0.18 |
| (1,3480) | 1:32:A:HIS:HD2 | 1:150:A:PRO:HG3 | 13 | 0.18 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 20 | 0.18 |
| (1,3418) | 1:59:A:TYR:HD1 | 1:75:A:TRP:HD1 | 11 | 0.18 |
| (1,3418) | 1:59:A:TYR:HD2 | 1:75:A:TRP:HD1 | 11 | 0.18 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD11 | 9 | 0.18 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD12 | 9 | 0.18 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD13 | 9 | 0.18 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD11 | 9 | 0.18 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD12 | 9 | 0.18 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD13 | 9 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3311) | 1:29:A:TYR:HD1 | 1:71:A:LEU:HB2 | 5 | 0.18 |
| (1,3311) | 1:29:A:TYR:HD2 | 1:71:A:LEU:HB2 | 5 | 0.18 |
| (1,3303) | 1:20:A:PRO:HG2 | 1:23:A:LEU:HB3 | 7 | 0.18 |
| (1,3303) | 1:20:A:PRO:HG3 | 1:23:A:LEU:HB3 | 7 | 0.18 |
| (1,3288) | 1:29:A:TYR:H | 1:30:A:CYS:HB2 | 7 | 0.18 |
| (1,3277) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA3 | 20 | 0.18 |
| (1,3277) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA3 | 20 | 0.18 |
| (1,3277) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA3 | 20 | 0.18 |
| (1,3229) | 1:88:A:THR:H | 1:90:A:PRO:HD3 | 12 | 0.18 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG21 | 14 | 0.18 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG22 | 14 | 0.18 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG23 | 14 | 0.18 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG21 | 14 | 0.18 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG22 | 14 | 0.18 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG23 | 14 | 0.18 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG21 | 14 | 0.18 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG22 | 14 | 0.18 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG23 | 14 | 0.18 |
| (1,3053) | 1:172:A:VAL:HG21 | 1:175:A:ALA:HB1 | 15 | 0.18 |
| (1,3053) | 1:172:A:VAL:HG21 | 1:175:A:ALA:HB2 | 15 | 0.18 |
| (1,3053) | 1:172:A:VAL:HG21 | 1:175:A:ALA:HB3 | 15 | 0.18 |
| (1,3053) | 1:172:A:VAL:HG22 | 1:175:A:ALA:HB1 | 15 | 0.18 |
| (1,3053) | 1:172:A:VAL:HG22 | 1:175:A:ALA:HB2 | 15 | 0.18 |
| (1,3053) | 1:172:A:VAL:HG22 | 1:175:A:ALA:HB3 | 15 | 0.18 |
| (1,3053) | 1:172:A:VAL:HG23 | 1:175:A:ALA:HB1 | 15 | 0.18 |
| (1,3053) | 1:172:A:VAL:HG23 | 1:175:A:ALA:HB2 | 15 | 0.18 |
| (1,3053) | 1:172:A:VAL:HG23 | 1:175:A:ALA:HB3 | 15 | 0.18 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 10 | 0.18 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 10 | 0.18 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 10 | 0.18 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 10 | 0.18 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 10 | 0.18 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 10 | 0.18 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 10 | 0.18 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 10 | 0.18 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 10 | 0.18 |
| (1,2987) | 1:50:A:LEU:HD21 | 1:56:A:MET:HA | 9 | 0.18 |
| (1,2987) | 1:50:A:LEU:HD22 | 1:56:A:MET:HA | 9 | 0.18 |
| (1,2987) | 1:50:A:LEU:HD23 | 1:56:A:MET:HA | 9 | 0.18 |
| (1,2935) | 1:75:A:TRP:HA | 1:78:A:ALA:HA | 7 | 0.18 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB1 | 18 | 0.18 |
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB2 | 18 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2933) | 1:175:A:ALA:HA | 1:178:A:ALA:HB3 | 18 | 0.18 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 6 | 0.18 |
| (1,2812) | 1:153:A:TYR:HA | 1:158:A:TYR:HB3 | 1 | 0.18 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD11 | 14 | 0.18 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD12 | 14 | 0.18 |
| (1,2810) | 1:25:A:PHE:HA | 1:146:A:LEU:HD13 | 14 | 0.18 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 15 | 0.18 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 15 | 0.18 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 15 | 0.18 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 20 | 0.18 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 20 | 0.18 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 20 | 0.18 |
| (1,2680) | 1:97:A:LYS:HA | 1:97:A:LYS:HD2 | 18 | 0.18 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG21 | 19 | 0.18 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG22 | 19 | 0.18 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG23 | 19 | 0.18 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG21 | 19 | 0.18 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG22 | 19 | 0.18 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG23 | 19 | 0.18 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG21 | 19 | 0.18 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG22 | 19 | 0.18 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG23 | 19 | 0.18 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG21 | 11 | 0.18 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG22 | 11 | 0.18 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG23 | 11 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD11 | 12 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD12 | 12 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD13 | 12 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD21 | 12 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD22 | 12 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD23 | 12 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD11 | 12 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD12 | 12 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD13 | 12 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD21 | 12 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD22 | 12 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD23 | 12 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD11 | 12 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD12 | 12 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD13 | 12 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD21 | 12 | 0.18 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD22 | 12 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD23 | 12 | 0.18 |
| (1,2621) | 1:101:A:VAL:HG21 | 1:106:A:ASP:H | 6 | 0.18 |
| (1,2621) | 1:101:A:VAL:HG22 | 1:106:A:ASP:H | 6 | 0.18 |
| (1,2621) | 1:101:A:VAL:HG23 | 1:106:A:ASP:H | 6 | 0.18 |
| (1,2621) | 1:101:A:VAL:HG21 | 1:106:A:ASP:H | 18 | 0.18 |
| (1,2621) | 1:101:A:VAL:HG22 | 1:106:A:ASP:H | 18 | 0.18 |
| (1,2621) | 1:101:A:VAL:HG23 | 1:106:A:ASP:H | 18 | 0.18 |
| (1,2602) | 1:47:A:ARG:HG2 | 1:48:A:GLN:HA | 11 | 0.18 |
| (1,2588) | 1:70:A:ASP:HA | 1:72:A:THR:H | 5 | 0.18 |
| (1,2581) | 1:52:A:GLU:HA | 1:53:A:GLY:HA3 | 2 | 0.18 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 13 | 0.18 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 13 | 0.18 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 13 | 0.18 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 2 | 0.18 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 10 | 0.18 |
| (1,2368) | 1:131:A:LYS:HA | 1:131:A:LYS:HG3 | 7 | 0.18 |
| (1,2347) | 1:131:A:LYS:HG3 | 1:131:A:LYS:HD2 | 9 | 0.18 |
| (1,2274) | 1:4:A:THR:HA | 1:7:A:LYS:HB2 | 5 | 0.18 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 16 | 0.18 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 16 | 0.18 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 16 | 0.18 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 16 | 0.18 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 16 | 0.18 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 16 | 0.18 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 14 | 0.18 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 7 | 0.18 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 7 | 0.18 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 2 | 0.18 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 2 | 0.18 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 2 | 0.18 |
| (1,2118) | 1:10:A:ILE:HG13 | 1:159:A:GLN:H | 15 | 0.18 |
| (1,2118) | 1:10:A:ILE:HG13 | 1:159:A:GLN:H | 16 | 0.18 |
| (1,2118) | 1:10:A:ILE:HG13 | 1:159:A:GLN:H | 19 | 0.18 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB2 | 20 | 0.18 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB3 | 20 | 0.18 |
| (1,2072) | 1:93:A:GLU:HA | 1:97:A:LYS:HD2 | 8 | 0.18 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 5 | 0.18 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 10 | 0.18 |
| (1,2020) | 1:86:A:LYS:H | 1:86:A:LYS:HD2 | 19 | 0.18 |
| (1,1981) | 1:187:A:LYS:H | 1:187:A:LYS:HD3 | 6 | 0.18 |
| (1,1981) | 1:187:A:LYS:H | 1:187:A:LYS:HD3 | 16 | 0.18 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 11 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 2 | 0.18 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG21 | 17 | 0.18 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG22 | 17 | 0.18 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG23 | 17 | 0.18 |
| (1,1912) | 1:32:A:HIS:HB3 | 1:34:A:TYR:H | 3 | 0.18 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 19 | 0.18 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 19 | 0.18 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 19 | 0.18 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 19 | 0.18 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 19 | 0.18 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 19 | 0.18 |
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 16 | 0.18 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 3 | 0.18 |
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 7 | 0.18 |
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 17 | 0.18 |
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 17 | 0.18 |
| (1,1778) | 1:72:A:THR:HB | 1:73:A:GLN:HB3 | 1 | 0.18 |
| (1,1758) | 1:14:A:LYS:H | 1:14:A:LYS:HB3 | 6 | 0.18 |
| (1,1758) | 1:14:A:LYS:H | 1:14:A:LYS:HB3 | 16 | 0.18 |
| (1,1730) | 1:55:A:LYS:H | 1:55:A:LYS:HB3 | 20 | 0.18 |
| (1,1685) | 1:99:A:GLN:HA | 1:99:A:GLN:HG3 | 9 | 0.18 |
| (1,1604) | 1:61:A:VAL:HA | 1:62:A:GLU:HG2 | 15 | 0.18 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 4 | 0.18 |
| (1,1526) | 1:63:A:PHE:HB2 | 1:64:A:LEU:H | 9 | 0.18 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 1 | 0.18 |
| (1,1474) | 1:161:A:ASN:HB2 | 1:161:A:ASN:HD22 | 1 | 0.18 |
| (1,1474) | 1:161:A:ASN:HB2 | 1:161:A:ASN:HD22 | 16 | 0.18 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG11 | 6 | 0.18 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG12 | 6 | 0.18 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG13 | 6 | 0.18 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG11 | 19 | 0.18 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG12 | 19 | 0.18 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG13 | 19 | 0.18 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG11 | 5 | 0.18 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG12 | 5 | 0.18 |
| (1,1442) | 1:45:A:ASN:HB2 | 1:46:A:VAL:HG13 | 5 | 0.18 |
| (1,1438) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HB2 | 2 | 0.18 |
| (1,1438) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HB2 | 2 | 0.18 |
| (1,1438) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HB2 | 2 | 0.18 |
| (1,1438) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HB2 | 19 | 0.18 |
| (1,1438) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HB2 | 19 | 0.18 |
| (1,1438) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HB2 | 19 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1426) | 1:143:A:ASP:HB2 | 1:144:A:LEU:HG | 9 | 0.18 |
| (1,1294) | 1:71:A:LEU:HB2 | 1:74:A:ALA:H | 6 | 0.18 |
| (1,1294) | 1:71:A:LEU:HB2 | 1:74:A:ALA:H | 18 | 0.18 |
| (1,1202) | 1:92:A:PHE:HD1 | 1:96:A:GLN:HE22 | 13 | 0.18 |
| (1,1202) | 1:92:A:PHE:HD2 | 1:96:A:GLN:HE22 | 13 | 0.18 |
| (1,1164) | 1:27:A:SER:H | 1:30:A:CYS:HB3 | 7 | 0.18 |
| (1,1164) | 1:27:A:SER:H | 1:30:A:CYS:HB3 | 11 | 0.18 |
| (1,1040) | 1:52:A:GLU:HB3 | 1:53:A:GLY:H | 5 | 0.18 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 7 | 0.18 |
| (1,1023) | 1:183:A:GLN:HG3 | 1:183:A:GLN:HE22 | 8 | 0.18 |
| (1,1005) | 1:46:A:VAL:HG21 | 1:48:A:GLN:H | 5 | 0.18 |
| (1,1005) | 1:46:A:VAL:HG22 | 1:48:A:GLN:H | 5 | 0.18 |
| (1,1005) | 1:46:A:VAL:HG23 | 1:48:A:GLN:H | 5 | 0.18 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG21 | 19 | 0.18 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG22 | 19 | 0.18 |
| (1,980) | 1:29:A:TYR:H | 1:95:A:VAL:HG23 | 19 | 0.18 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 15 | 0.18 |
| (1,967) | 1:126:A:ASN:HB2 | 1:126:A:ASN:HD22 | 3 | 0.18 |
| (1,966) | 1:122:A:ASP:HA | 1:126:A:ASN:HD22 | 19 | 0.18 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 18 | 0.18 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 18 | 0.18 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 18 | 0.18 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 6 | 0.18 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 8 | 0.18 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 16 | 0.18 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 5 | 0.18 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 5 | 0.18 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 5 | 0.18 |
| (1,815) | 1:91:A:MET:HB2 | 1:93:A:GLU:H | 20 | 0.18 |
| (1,749) | 1:117:A:LYS:HB2 | 1:119:A:GLU:H | 11 | 0.18 |
| (1,669) | 1:108:A:ARG:H | 1:108:A:ARG:HB2 | 6 | 0.18 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 10 | 0.18 |
| (1,568) | 1:49:A:LYS:HA | 1:50:A:LEU:H | 2 | 0.18 |
| (1,568) | 1:49:A:LYS:HA | 1:50:A:LEU:H | 16 | 0.18 |
| (1,560) | 1:42:A:VAL:HG21 | 1:178:A:ALA:H | 11 | 0.18 |
| (1,560) | 1:42:A:VAL:HG22 | 1:178:A:ALA:H | 11 | 0.18 |
| (1,560) | 1:42:A:VAL:HG23 | 1:178:A:ALA:H | 11 | 0.18 |
| (1,555) | 1:174:A:VAL:HG21 | 1:178:A:ALA:H | 14 | 0.18 |
| (1,555) | 1:174:A:VAL:HG22 | 1:178:A:ALA:H | 14 | 0.18 |
| (1,555) | 1:174:A:VAL:HG23 | 1:178:A:ALA:H | 14 | 0.18 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 8 | 0.18 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 8 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 8 | 0.18 |
| (1,498) | 1:77:A:VAL:HG11 | 1:124:A:ALA:H | 10 | 0.18 |
| (1,498) | 1:77:A:VAL:HG12 | 1:124:A:ALA:H | 10 | 0.18 |
| (1,498) | 1:77:A:VAL:HG13 | 1:124:A:ALA:H | 10 | 0.18 |
| (1,492) | 1:138:A:GLU:HB2 | 1:140:A:ALA:H | 17 | 0.18 |
| (1,438) | 1:60:A:HIS:HB2 | 1:75:A:TRP:H | 16 | 0.18 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 20 | 0.18 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 20 | 0.18 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 20 | 0.18 |
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 5 | 0.18 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 1 | 0.18 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 7 | 0.18 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 18 | 0.18 |
| (1,216) | 1:34:A:TYR:H | 1:96:A:GLN:HE21 | 19 | 0.18 |
| (1,185) | 1:59:A:TYR:HB2 | 1:60:A:HIS:H | 5 | 0.18 |
| (1,165) | 1:67:A:LEU:H | 1:69:A:LYS:H | 1 | 0.18 |
| (1,165) | 1:67:A:LEU:H | 1:69:A:LYS:H | 16 | 0.18 |
| (1,164) | 1:69:A:LYS:H | 1:69:A:LYS:HB3 | 8 | 0.18 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD21 | 5 | 0.18 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD22 | 5 | 0.18 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD23 | 5 | 0.18 |
| (1,103) | 1:55:A:LYS:HB2 | 1:56:A:MET:H | 1 | 0.18 |
| (1,83) | 1:6:A:GLY:H | 1:11:A:THR:H | 3 | 0.18 |
| (1,67) | 1:26:A:PHE:H | 1:59:A:TYR:H | 12 | 0.18 |
| (1,63) | 1:102:A:GLN:H | 1:102:A:GLN:HB3 | 19 | 0.18 |
| (1,3523) | 1:73:A:GLN:HE21 | 1:125:A:TRP:HZ2 | 6 | 0.17 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 10 | 0.17 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 10 | 0.17 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 10 | 0.17 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 10 | 0.17 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 10 | 0.17 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 10 | 0.17 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 14 | 0.17 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 14 | 0.17 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 14 | 0.17 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 14 | 0.17 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 14 | 0.17 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 14 | 0.17 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE1 | 14 | 0.17 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE2 | 14 | 0.17 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE1 | 14 | 0.17 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE2 | 14 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE1 | 17 | 0.17 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE2 | 17 | 0.17 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE1 | 17 | 0.17 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE2 | 17 | 0.17 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB2 | 14 | 0.17 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB3 | 14 | 0.17 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB2 | 14 | 0.17 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB3 | 14 | 0.17 |
| (1,3487) | 1:29:A:TYR:HE1 | 1:67:A:LEU:H | 7 | 0.17 |
| (1,3487) | 1:29:A:TYR:HE2 | 1:67:A:LEU:H | 7 | 0.17 |
| (1,3461) | 1:75:A:TRP:HB3 | 1:75:A:TRP:HE3 | 5 | 0.17 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 4 | 0.17 |
| (1,3430) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HB3 | 9 | 0.17 |
| (1,3419) | 1:75:A:TRP:HB2 | 1:75:A:TRP:HD1 | 20 | 0.17 |
| (1,3398) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HG2 | 1 | 0.17 |
| (1,3398) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HG3 | 1 | 0.17 |
| (1,3398) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HG2 | 1 | 0.17 |
| (1,3398) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HG3 | 1 | 0.17 |
| (1,3389) | 1:128:A:PHE:HD2 | 1:131:A:LYS:HB2 | 11 | 0.17 |
| (1,3389) | 1:128:A:PHE:HD2 | 1:131:A:LYS:HB3 | 11 | 0.17 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD11 | 7 | 0.17 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD12 | 7 | 0.17 |
| (1,3354) | 1:63:A:PHE:HD1 | 1:64:A:LEU:HD13 | 7 | 0.17 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD11 | 7 | 0.17 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD12 | 7 | 0.17 |
| (1,3354) | 1:63:A:PHE:HD2 | 1:64:A:LEU:HD13 | 7 | 0.17 |
| (1,3345) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 2 | 0.17 |
| (1,3345) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 2 | 0.17 |
| (1,3345) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 2 | 0.17 |
| (1,3345) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 2 | 0.17 |
| (1,3345) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 2 | 0.17 |
| (1,3345) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 2 | 0.17 |
| (1,3345) | 1:46:A:VAL:HG21 | 1:177:A:TYR:HD1 | 2 | 0.17 |
| (1,3345) | 1:46:A:VAL:HG21 | 1:177:A:TYR:HD2 | 2 | 0.17 |
| (1,3345) | 1:46:A:VAL:HG22 | 1:177:A:TYR:HD1 | 2 | 0.17 |
| (1,3345) | 1:46:A:VAL:HG22 | 1:177:A:TYR:HD2 | 2 | 0.17 |
| (1,3345) | 1:46:A:VAL:HG23 | 1:177:A:TYR:HD1 | 2 | 0.17 |
| (1,3345) | 1:46:A:VAL:HG23 | 1:177:A:TYR:HD2 | 2 | 0.17 |
| (1,3277) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA3 | 4 | 0.17 |
| (1,3277) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA3 | 4 | 0.17 |
| (1,3277) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA3 | 4 | 0.17 |
| (1,3274) | 1:118:A:GLY:HA3 | 1:121:A:TYR:H | 16 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3269) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA2 | 5 | 0.17 |
| (1,3269) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA2 | 5 | 0.17 |
| (1,3269) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA2 | 5 | 0.17 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE1 | 16 | 0.17 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE2 | 16 | 0.17 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE3 | 16 | 0.17 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG21 | 16 | 0.17 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG22 | 16 | 0.17 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG23 | 16 | 0.17 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG21 | 16 | 0.17 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG22 | 16 | 0.17 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG23 | 16 | 0.17 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG21 | 16 | 0.17 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG22 | 16 | 0.17 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG23 | 16 | 0.17 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG21 | 18 | 0.17 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG22 | 18 | 0.17 |
| (1,3066) | 1:61:A:VAL:HG21 | 1:72:A:THR:HG23 | 18 | 0.17 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG21 | 18 | 0.17 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG22 | 18 | 0.17 |
| (1,3066) | 1:61:A:VAL:HG22 | 1:72:A:THR:HG23 | 18 | 0.17 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG21 | 18 | 0.17 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG22 | 18 | 0.17 |
| (1,3066) | 1:61:A:VAL:HG23 | 1:72:A:THR:HG23 | 18 | 0.17 |
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 18 | 0.17 |
| (1,2945) | 1:23:A:LEU:HD21 | 1:58:A:LYS:HA | 7 | 0.17 |
| (1,2945) | 1:23:A:LEU:HD22 | 1:58:A:LYS:HA | 7 | 0.17 |
| (1,2945) | 1:23:A:LEU:HD23 | 1:58:A:LYS:HA | 7 | 0.17 |
| (1,2943) | 1:3:A:ILE:HG21 | 1:8:A:GLN:HG3 | 8 | 0.17 |
| (1,2943) | 1:3:A:ILE:HG22 | 1:8:A:GLN:HG3 | 8 | 0.17 |
| (1,2943) | 1:3:A:ILE:HG23 | 1:8:A:GLN:HG3 | 8 | 0.17 |
| (1,2935) | 1:75:A:TRP:HA | 1:78:A:ALA:HA | 14 | 0.17 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 8 | 0.17 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 19 | 0.17 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 6 | 0.17 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 6 | 0.17 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 6 | 0.17 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 16 | 0.17 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 16 | 0.17 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 16 | 0.17 |
| (1,2832) | 1:55:A:LYS:HA | 1:56:A:MET:HB2 | 12 | 0.17 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 3 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 3 | 0.17 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 3 | 0.17 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 3 | 0.17 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 3 | 0.17 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 3 | 0.17 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 3 | 0.17 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 3 | 0.17 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 3 | 0.17 |
| (1,2779) | 1:62:A:GLU:HA | 1:69:A:LYS:H | 7 | 0.17 |
| (1,2753) | 1:61:A:VAL:HG11 | 1:62:A:GLU:HA | 18 | 0.17 |
| (1,2753) | 1:61:A:VAL:HG12 | 1:62:A:GLU:HA | 18 | 0.17 |
| (1,2753) | 1:61:A:VAL:HG13 | 1:62:A:GLU:HA | 18 | 0.17 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 13 | 0.17 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 13 | 0.17 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 13 | 0.17 |
| (1,2699) | 1:134:A:VAL:HG11 | 1:138:A:GLU:HG3 | 17 | 0.17 |
| (1,2699) | 1:134:A:VAL:HG12 | 1:138:A:GLU:HG3 | 17 | 0.17 |
| (1,2699) | 1:134:A:VAL:HG13 | 1:138:A:GLU:HG3 | 17 | 0.17 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG21 | 13 | 0.17 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG22 | 13 | 0.17 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG23 | 13 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG21 | 9 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG22 | 9 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG23 | 9 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG21 | 9 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG22 | 9 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG23 | 9 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG21 | 9 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG22 | 9 | 0.17 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG23 | 9 | 0.17 |
| (1,2622) | 1:149:A:VAL:HA | 1:151:A:ALA:H | 19 | 0.17 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 17 | 0.17 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 17 | 0.17 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 17 | 0.17 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 17 | 0.17 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 17 | 0.17 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 17 | 0.17 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 1 | 0.17 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 1 | 0.17 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 1 | 0.17 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 2 | 0.17 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 2 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 2 | 0.17 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 2 | 0.17 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 2 | 0.17 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 2 | 0.17 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 2 | 0.17 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 2 | 0.17 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 2 | 0.17 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 17 | 0.17 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 17 | 0.17 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 17 | 0.17 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 17 | 0.17 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 17 | 0.17 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 17 | 0.17 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 17 | 0.17 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 17 | 0.17 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 17 | 0.17 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD21 | 7 | 0.17 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD22 | 7 | 0.17 |
| (1,2557) | 1:39:A:VAL:HB | 1:40:A:LEU:HD23 | 7 | 0.17 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG21 | 7 | 0.17 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG22 | 7 | 0.17 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG23 | 7 | 0.17 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG21 | 7 | 0.17 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG22 | 7 | 0.17 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG23 | 7 | 0.17 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG21 | 7 | 0.17 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG22 | 7 | 0.17 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG23 | 7 | 0.17 |
| (1,2535) | 1:20:A:PRO:HG2 | 1:57:A:THR:HG21 | 15 | 0.17 |
| (1,2535) | 1:20:A:PRO:HG2 | 1:57:A:THR:HG22 | 15 | 0.17 |
| (1,2535) | 1:20:A:PRO:HG2 | 1:57:A:THR:HG23 | 15 | 0.17 |
| (1,2535) | 1:20:A:PRO:HG3 | 1:57:A:THR:HG21 | 15 | 0.17 |
| (1,2535) | 1:20:A:PRO:HG3 | 1:57:A:THR:HG22 | 15 | 0.17 |
| (1,2535) | 1:20:A:PRO:HG3 | 1:57:A:THR:HG23 | 15 | 0.17 |
| (1,2529) | 1:97:A:LYS:H | 1:98:A:THR:HG21 | 7 | 0.17 |
| (1,2529) | 1:97:A:LYS:H | 1:98:A:THR:HG22 | 7 | 0.17 |
| (1,2529) | 1:97:A:LYS:H | 1:98:A:THR:HG23 | 7 | 0.17 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 14 | 0.17 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 16 | 0.17 |
| (1,2395) | 1:157:A:LYS:HG2 | 1:158:A:TYR:H | 7 | 0.17 |
| (1,2315) | 1:46:A:VAL:HG21 | 1:50:A:LEU:HG | 12 | 0.17 |
| (1,2315) | 1:46:A:VAL:HG22 | 1:50:A:LEU:HG | 12 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2315) | 1:46:A:VAL:HG23 | 1:50:A:LEU:HG | 12 | 0.17 |
| (1,2226) | 1:111:A:PHE:HA | 1:116:A:VAL:HG11 | 14 | 0.17 |
| (1,2226) | 1:111:A:PHE:HA | 1:116:A:VAL:HG12 | 14 | 0.17 |
| (1,2226) | 1:111:A:PHE:HA | 1:116:A:VAL:HG13 | 14 | 0.17 |
| (1,2159) | 1:76:A:ALA:HA | 1:79:A:ILE:HG12 | 13 | 0.17 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 14 | 0.17 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 14 | 0.17 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 14 | 0.17 |
| (1,2072) | 1:93:A:GLU:HA | 1:97:A:LYS:HD2 | 17 | 0.17 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 20 | 0.17 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD1 | 1 | 0.17 |
| (1,2043) | 1:27:A:SER:HB2 | 1:29:A:TYR:HD2 | 1 | 0.17 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG11 | 19 | 0.17 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG12 | 19 | 0.17 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG13 | 19 | 0.17 |
| (1,2000) | 1:187:A:LYS:HA | 1:187:A:LYS:HD3 | 8 | 0.17 |
| (1,1989) | 1:136:A:GLN:HB2 | 1:137:A:GLN:H | 17 | 0.17 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 16 | 0.17 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 20 | 0.17 |
| (1,1915) | 1:186:A:GLU:HB2 | 1:187:A:LYS:H | 3 | 0.17 |
| (1,1915) | 1:186:A:GLU:HB2 | 1:187:A:LYS:H | 5 | 0.17 |
| (1,1915) | 1:186:A:GLU:HB2 | 1:187:A:LYS:H | 13 | 0.17 |
| (1,1912) | 1:32:A:HIS:HB3 | 1:34:A:TYR:H | 13 | 0.17 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB2 | 14 | 0.17 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB3 | 14 | 0.17 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB2 | 14 | 0.17 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB3 | 14 | 0.17 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB2 | 14 | 0.17 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB3 | 14 | 0.17 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD21 | 11 | 0.17 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD22 | 11 | 0.17 |
| (1,1906) | 1:47:A:ARG:HB2 | 1:50:A:LEU:HD23 | 11 | 0.17 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD21 | 11 | 0.17 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD22 | 11 | 0.17 |
| (1,1906) | 1:47:A:ARG:HB3 | 1:50:A:LEU:HD23 | 11 | 0.17 |
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 10 | 0.17 |
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 14 | 0.17 |
| (1,1832) | 1:124:A:ALA:HB1 | 1:130:A:VAL:HB | 6 | 0.17 |
| (1,1832) | 1:124:A:ALA:HB2 | 1:130:A:VAL:HB | 6 | 0.17 |
| (1,1832) | 1:124:A:ALA:HB3 | 1:130:A:VAL:HB | 6 | 0.17 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 20 | 0.17 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD1 | 3 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD2 | 3 | 0.17 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD1 | 17 | 0.17 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD2 | 17 | 0.17 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD1 | 19 | 0.17 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD2 | 19 | 0.17 |
| (1,1785) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD2 | 2 | 0.17 |
| (1,1785) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD2 | 13 | 0.17 |
| (1,1758) | 1:14:A:LYS:H | 1:14:A:LYS:HB3 | 7 | 0.17 |
| (1,1758) | 1:14:A:LYS:H | 1:14:A:LYS:HB3 | 13 | 0.17 |
| (1,1730) | 1:55:A:LYS:H | 1:55:A:LYS:HB3 | 6 | 0.17 |
| (1,1730) | 1:55:A:LYS:H | 1:55:A:LYS:HB3 | 10 | 0.17 |
| (1,1695) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HE22 | 11 | 0.17 |
| (1,1694) | 1:136:A:GLN:HG2 | 1:137:A:GLN:H | 16 | 0.17 |
| (1,1685) | 1:99:A:GLN:HA | 1:99:A:GLN:HG3 | 5 | 0.17 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 9 | 0.17 |
| (1,1552) | 1:186:A:GLU:HB2 | 1:186:A:GLU:HG2 | 7 | 0.17 |
| (1,1533) | 1:34:A:TYR:HB3 | 1:96:A:GLN:HE21 | 3 | 0.17 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG11 | 18 | 0.17 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG12 | 18 | 0.17 |
| (1,1502) | 1:111:A:PHE:HB3 | 1:112:A:VAL:HG13 | 18 | 0.17 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 2 | 0.17 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 2 | 0.17 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 2 | 0.17 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 19 | 0.17 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 19 | 0.17 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 19 | 0.17 |
| (1,1474) | 1:161:A:ASN:HB2 | 1:161:A:ASN:HD22 | 15 | 0.17 |
| (1,1438) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HB2 | 6 | 0.17 |
| (1,1438) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HB2 | 6 | 0.17 |
| (1,1438) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HB2 | 6 | 0.17 |
| (1,1431) | 1:85:A:ASP:HB3 | 1:87:A:ILE:H | 18 | 0.17 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG11 | 14 | 0.17 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG12 | 14 | 0.17 |
| (1,1425) | 1:171:A:ASP:HB3 | 1:172:A:VAL:HG13 | 14 | 0.17 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 5 | 0.17 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 5 | 0.17 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 5 | 0.17 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB2 | 10 | 0.17 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB3 | 10 | 0.17 |
| (1,1366) | 1:34:A:TYR:HE1 | 1:97:A:LYS:HE3 | 9 | 0.17 |
| (1,1366) | 1:34:A:TYR:HE2 | 1:97:A:LYS:HE3 | 9 | 0.17 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE2 | 6 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE3 | 6 | 0.17 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE2 | 6 | 0.17 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE3 | 6 | 0.17 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE2 | 6 | 0.17 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE3 | 6 | 0.17 |
| (1,1354) | 1:73:A:GLN:HE22 | 1:131:A:LYS:HE2 | 13 | 0.17 |
| (1,1354) | 1:73:A:GLN:HE22 | 1:131:A:LYS:HE3 | 13 | 0.17 |
| (1,1298) | 1:141:A:ALA:HA | 1:146:A:LEU:HB2 | 9 | 0.17 |
| (1,1265) | 1:64:A:LEU:HB3 | 1:65:A:GLY:HA2 | 17 | 0.17 |
| (1,1258) | 1:163:A:GLN:HG2 | 1:164:A:GLY:HA3 | 1 | 0.17 |
| (1,1258) | 1:163:A:GLN:HG3 | 1:164:A:GLY:HA3 | 1 | 0.17 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG11 | 12 | 0.17 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG12 | 12 | 0.17 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG13 | 12 | 0.17 |
| (1,1164) | 1:27:A:SER:H | 1:30:A:CYS:HB3 | 3 | 0.17 |
| (1,1109) | 1:40:A:LEU:HD11 | 1:41:A:HIS:H | 16 | 0.17 |
| (1,1109) | 1:40:A:LEU:HD12 | 1:41:A:HIS:H | 16 | 0.17 |
| (1,1109) | 1:40:A:LEU:HD13 | 1:41:A:HIS:H | 16 | 0.17 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 10 | 0.17 |
| (1,1005) | 1:46:A:VAL:HG21 | 1:48:A:GLN:H | 19 | 0.17 |
| (1,1005) | 1:46:A:VAL:HG22 | 1:48:A:GLN:H | 19 | 0.17 |
| (1,1005) | 1:46:A:VAL:HG23 | 1:48:A:GLN:H | 19 | 0.17 |
| (1,991) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HD22 | 4 | 0.17 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 5 | 0.17 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 6 | 0.17 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 10 | 0.17 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 11 | 0.17 |
| (1,967) | 1:126:A:ASN:HB2 | 1:126:A:ASN:HD22 | 14 | 0.17 |
| (1,967) | 1:126:A:ASN:HB2 | 1:126:A:ASN:HD22 | 16 | 0.17 |
| (1,926) | 1:183:A:GLN:H | 1:183:A:GLN:HE22 | 19 | 0.17 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 2 | 0.17 |
| (1,883) | 1:49:A:LYS:H | 1:49:A:LYS:HD3 | 15 | 0.17 |
| (1,815) | 1:91:A:MET:HB2 | 1:93:A:GLU:H | 12 | 0.17 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 9 | 0.17 |
| (1,732) | 1:95:A:VAL:HG21 | 1:97:A:LYS:H | 2 | 0.17 |
| (1,732) | 1:95:A:VAL:HG22 | 1:97:A:LYS:H | 2 | 0.17 |
| (1,732) | 1:95:A:VAL:HG23 | 1:97:A:LYS:H | 2 | 0.17 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 6 | 0.17 |
| (1,678) | 1:71:A:LEU:HD21 | 1:72:A:THR:H | 10 | 0.17 |
| (1,678) | 1:71:A:LEU:HD22 | 1:72:A:THR:H | 10 | 0.17 |
| (1,678) | 1:71:A:LEU:HD23 | 1:72:A:THR:H | 10 | 0.17 |
| (1,650) | 1:145:A:GLN:HA | 1:146:A:LEU:H | 4 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 20 | 0.17 |
| (1,599) | 1:183:A:GLN:HB3 | 1:184:A:LEU:H | 7 | 0.17 |
| (1,599) | 1:183:A:GLN:HB3 | 1:184:A:LEU:H | 20 | 0.17 |
| (1,577) | 1:121:A:TYR:HB2 | 1:122:A:ASP:H | 6 | 0.17 |
| (1,568) | 1:49:A:LYS:HA | 1:50:A:LEU:H | 1 | 0.17 |
| (1,568) | 1:49:A:LYS:HA | 1:50:A:LEU:H | 5 | 0.17 |
| (1,568) | 1:49:A:LYS:HA | 1:50:A:LEU:H | 8 | 0.17 |
| (1,568) | 1:49:A:LYS:HA | 1:50:A:LEU:H | 18 | 0.17 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG21 | 7 | 0.17 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG22 | 7 | 0.17 |
| (1,499) | 1:124:A:ALA:H | 1:130:A:VAL:HG23 | 7 | 0.17 |
| (1,485) | 1:4:A:THR:H | 1:7:A:LYS:HB2 | 12 | 0.17 |
| (1,300) | 1:130:A:VAL:HG21 | 1:131:A:LYS:H | 6 | 0.17 |
| (1,300) | 1:130:A:VAL:HG22 | 1:131:A:LYS:H | 6 | 0.17 |
| (1,300) | 1:130:A:VAL:HG23 | 1:131:A:LYS:H | 6 | 0.17 |
| (1,300) | 1:130:A:VAL:HG21 | 1:131:A:LYS:H | 15 | 0.17 |
| (1,300) | 1:130:A:VAL:HG22 | 1:131:A:LYS:H | 15 | 0.17 |
| (1,300) | 1:130:A:VAL:HG23 | 1:131:A:LYS:H | 15 | 0.17 |
| (1,165) | 1:67:A:LEU:H | 1:69:A:LYS:H | 12 | 0.17 |
| (1,165) | 1:67:A:LEU:H | 1:69:A:LYS:H | 15 | 0.17 |
| (1,132) | 1:56:A:MET:HB2 | 1:57:A:THR:H | 20 | 0.17 |
| (1,62) | 1:102:A:GLN:H | 1:102:A:GLN:HG2 | 12 | 0.17 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE1 | 18 | 0.16 |
| (1,3516) | 1:160:A:LEU:HD21 | 1:177:A:TYR:HE2 | 18 | 0.16 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE1 | 18 | 0.16 |
| (1,3516) | 1:160:A:LEU:HD22 | 1:177:A:TYR:HE2 | 18 | 0.16 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE1 | 18 | 0.16 |
| (1,3516) | 1:160:A:LEU:HD23 | 1:177:A:TYR:HE2 | 18 | 0.16 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE1 | 4 | 0.16 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE2 | 4 | 0.16 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE1 | 15 | 0.16 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE2 | 15 | 0.16 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE1 | 15 | 0.16 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE2 | 15 | 0.16 |
| (1,3484) | 1:29:A:TYR:HE1 | 1:68:A:GLY:HA3 | 15 | 0.16 |
| (1,3484) | 1:29:A:TYR:HE2 | 1:68:A:GLY:HA3 | 15 | 0.16 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE1 | 16 | 0.16 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE2 | 16 | 0.16 |
| (1,3461) | 1:75:A:TRP:HB3 | 1:75:A:TRP:HE3 | 17 | 0.16 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 8 | 0.16 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG2 | 5 | 0.16 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG3 | 5 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3430) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HB3 | 6 | 0.16 |
| (1,3419) | 1:75:A:TRP:HB2 | 1:75:A:TRP:HD1 | 12 | 0.16 |
| (1,3419) | 1:75:A:TRP:HB2 | 1:75:A:TRP:HD1 | 13 | 0.16 |
| (1,3417) | 1:36:A:PHE:HD1 | 1:42:A:VAL:HG11 | 10 | 0.16 |
| (1,3417) | 1:36:A:PHE:HD1 | 1:42:A:VAL:HG12 | 10 | 0.16 |
| (1,3417) | 1:36:A:PHE:HD1 | 1:42:A:VAL:HG13 | 10 | 0.16 |
| (1,3417) | 1:36:A:PHE:HD2 | 1:42:A:VAL:HG11 | 10 | 0.16 |
| (1,3417) | 1:36:A:PHE:HD2 | 1:42:A:VAL:HG12 | 10 | 0.16 |
| (1,3417) | 1:36:A:PHE:HD2 | 1:42:A:VAL:HG13 | 10 | 0.16 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD11 | 5 | 0.16 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD12 | 5 | 0.16 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD13 | 5 | 0.16 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD11 | 5 | 0.16 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD12 | 5 | 0.16 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD13 | 5 | 0.16 |
| (1,3415) | 1:59:A:TYR:HD1 | 1:137:A:GLN:HG3 | 15 | 0.16 |
| (1,3415) | 1:59:A:TYR:HD2 | 1:137:A:GLN:HG3 | 15 | 0.16 |
| (1,3404) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HB2 | 11 | 0.16 |
| (1,3404) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HB3 | 11 | 0.16 |
| (1,3404) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HB2 | 11 | 0.16 |
| (1,3404) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HB3 | 11 | 0.16 |
| (1,3398) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HG2 | 10 | 0.16 |
| (1,3398) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HG3 | 10 | 0.16 |
| (1,3398) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HG2 | 10 | 0.16 |
| (1,3398) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HG3 | 10 | 0.16 |
| (1,3389) | 1:128:A:PHE:HD2 | 1:131:A:LYS:HB2 | 3 | 0.16 |
| (1,3389) | 1:128:A:PHE:HD2 | 1:131:A:LYS:HB3 | 3 | 0.16 |
| (1,3389) | 1:128:A:PHE:HD2 | 1:131:A:LYS:HB2 | 5 | 0.16 |
| (1,3389) | 1:128:A:PHE:HD2 | 1:131:A:LYS:HB3 | 5 | 0.16 |
| (1,3389) | 1:128:A:PHE:HD2 | 1:131:A:LYS:HB2 | 9 | 0.16 |
| (1,3389) | 1:128:A:PHE:HD2 | 1:131:A:LYS:HB3 | 9 | 0.16 |
| (1,3378) | 1:40:A:LEU:HD11 | 1:173:A:PHE:HD1 | 15 | 0.16 |
| (1,3378) | 1:40:A:LEU:HD11 | 1:173:A:PHE:HD2 | 15 | 0.16 |
| (1,3378) | 1:40:A:LEU:HD12 | 1:173:A:PHE:HD1 | 15 | 0.16 |
| (1,3378) | 1:40:A:LEU:HD12 | 1:173:A:PHE:HD2 | 15 | 0.16 |
| (1,3378) | 1:40:A:LEU:HD13 | 1:173:A:PHE:HD1 | 15 | 0.16 |
| (1,3378) | 1:40:A:LEU:HD13 | 1:173:A:PHE:HD2 | 15 | 0.16 |
| (1,3376) | 1:34:A:TYR:HD1 | 1:38:A:GLU:HB3 | 14 | 0.16 |
| (1,3376) | 1:34:A:TYR:HD2 | 1:38:A:GLU:HB3 | 14 | 0.16 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD1 | 6 | 0.16 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD2 | 6 | 0.16 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD1 | 6 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD2 | 6 | 0.16 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD1 | 6 | 0.16 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD2 | 6 | 0.16 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD1 | 13 | 0.16 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD2 | 13 | 0.16 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD1 | 13 | 0.16 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD2 | 13 | 0.16 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD1 | 13 | 0.16 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD2 | 13 | 0.16 |
| (1,3336) | 1:92:A:PHE:HD1 | 1:96:A:GLN:HG2 | 11 | 0.16 |
| (1,3336) | 1:92:A:PHE:HD2 | 1:96:A:GLN:HG2 | 11 | 0.16 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD1 | 2 | 0.16 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD2 | 2 | 0.16 |
| (1,3297) | 1:23:A:LEU:HB2 | 1:153:A:TYR:H | 9 | 0.16 |
| (1,3277) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA3 | 19 | 0.16 |
| (1,3277) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA3 | 19 | 0.16 |
| (1,3277) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA3 | 19 | 0.16 |
| (1,3274) | 1:118:A:GLY:HA3 | 1:121:A:TYR:H | 8 | 0.16 |
| (1,3252) | 1:29:A:TYR:HD1 | 1:68:A:GLY:HA3 | 12 | 0.16 |
| (1,3252) | 1:29:A:TYR:HD2 | 1:68:A:GLY:HA3 | 12 | 0.16 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD11 | 18 | 0.16 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD12 | 18 | 0.16 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD13 | 18 | 0.16 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD11 | 18 | 0.16 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD12 | 18 | 0.16 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD13 | 18 | 0.16 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD11 | 18 | 0.16 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD12 | 18 | 0.16 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD13 | 18 | 0.16 |
| (1,3053) | 1:172:A:VAL:HG21 | 1:175:A:ALA:HB1 | 16 | 0.16 |
| (1,3053) | 1:172:A:VAL:HG21 | 1:175:A:ALA:HB2 | 16 | 0.16 |
| (1,3053) | 1:172:A:VAL:HG21 | 1:175:A:ALA:HB3 | 16 | 0.16 |
| (1,3053) | 1:172:A:VAL:HG22 | 1:175:A:ALA:HB1 | 16 | 0.16 |
| (1,3053) | 1:172:A:VAL:HG22 | 1:175:A:ALA:HB2 | 16 | 0.16 |
| (1,3053) | 1:172:A:VAL:HG22 | 1:175:A:ALA:HB3 | 16 | 0.16 |
| (1,3053) | 1:172:A:VAL:HG23 | 1:175:A:ALA:HB1 | 16 | 0.16 |
| (1,3053) | 1:172:A:VAL:HG23 | 1:175:A:ALA:HB2 | 16 | 0.16 |
| (1,3053) | 1:172:A:VAL:HG23 | 1:175:A:ALA:HB3 | 16 | 0.16 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 12 | 0.16 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 12 | 0.16 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 12 | 0.16 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 12 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 12 | 0.16 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 12 | 0.16 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 12 | 0.16 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 12 | 0.16 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 12 | 0.16 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 12 | 0.16 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 12 | 0.16 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 12 | 0.16 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 12 | 0.16 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 12 | 0.16 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 12 | 0.16 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 12 | 0.16 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 12 | 0.16 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 12 | 0.16 |
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 16 | 0.16 |
| (1,2935) | 1:75:A:TRP:HA | 1:78:A:ALA:HA | 2 | 0.16 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 7 | 0.16 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 6 | 0.16 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 10 | 0.16 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 16 | 0.16 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 17 | 0.16 |
| (1,2838) | 1:34:A:TYR:HE1 | 1:38:A:GLU:HA | 1 | 0.16 |
| (1,2838) | 1:34:A:TYR:HE2 | 1:38:A:GLU:HA | 1 | 0.16 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 5 | 0.16 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 5 | 0.16 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 5 | 0.16 |
| (1,2753) | 1:61:A:VAL:HG11 | 1:62:A:GLU:HA | 9 | 0.16 |
| (1,2753) | 1:61:A:VAL:HG12 | 1:62:A:GLU:HA | 9 | 0.16 |
| (1,2753) | 1:61:A:VAL:HG13 | 1:62:A:GLU:HA | 9 | 0.16 |
| (1,2753) | 1:61:A:VAL:HG11 | 1:62:A:GLU:HA | 10 | 0.16 |
| (1,2753) | 1:61:A:VAL:HG12 | 1:62:A:GLU:HA | 10 | 0.16 |
| (1,2753) | 1:61:A:VAL:HG13 | 1:62:A:GLU:HA | 10 | 0.16 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG11 | 8 | 0.16 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG12 | 8 | 0.16 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG13 | 8 | 0.16 |
| (1,2724) | 1:124:A:ALA:HA | 1:130:A:VAL:HG11 | 7 | 0.16 |
| (1,2724) | 1:124:A:ALA:HA | 1:130:A:VAL:HG12 | 7 | 0.16 |
| (1,2724) | 1:124:A:ALA:HA | 1:130:A:VAL:HG13 | 7 | 0.16 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG21 | 14 | 0.16 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG22 | 14 | 0.16 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG23 | 14 | 0.16 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG21 | 14 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG22 | 14 | 0.16 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG23 | 14 | 0.16 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG21 | 14 | 0.16 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG22 | 14 | 0.16 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG23 | 14 | 0.16 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG21 | 2 | 0.16 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG22 | 2 | 0.16 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG23 | 2 | 0.16 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG21 | 4 | 0.16 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG22 | 4 | 0.16 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG23 | 4 | 0.16 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG21 | 19 | 0.16 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG22 | 19 | 0.16 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG23 | 19 | 0.16 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG21 | 19 | 0.16 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG22 | 19 | 0.16 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG23 | 19 | 0.16 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG21 | 19 | 0.16 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG22 | 19 | 0.16 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG23 | 19 | 0.16 |
| (1,2636) | 1:101:A:VAL:HG21 | 1:106:A:ASP:HB3 | 7 | 0.16 |
| (1,2636) | 1:101:A:VAL:HG22 | 1:106:A:ASP:HB3 | 7 | 0.16 |
| (1,2636) | 1:101:A:VAL:HG23 | 1:106:A:ASP:HB3 | 7 | 0.16 |
| (1,2622) | 1:149:A:VAL:HA | 1:151:A:ALA:H | 8 | 0.16 |
| (1,2596) | 1:63:A:PHE:HA | 1:64:A:LEU:H | 15 | 0.16 |
| (1,2474) | 1:83:A:VAL:HA | 1:84:A:GLU:HB2 | 1 | 0.16 |
| (1,2454) | 1:46:A:VAL:HG11 | 1:178:A:ALA:H | 14 | 0.16 |
| (1,2454) | 1:46:A:VAL:HG12 | 1:178:A:ALA:H | 14 | 0.16 |
| (1,2454) | 1:46:A:VAL:HG13 | 1:178:A:ALA:H | 14 | 0.16 |
| (1,2417) | 1:73:A:GLN:HA | 1:77:A:VAL:HG21 | 19 | 0.16 |
| (1,2417) | 1:73:A:GLN:HA | 1:77:A:VAL:HG22 | 19 | 0.16 |
| (1,2417) | 1:73:A:GLN:HA | 1:77:A:VAL:HG23 | 19 | 0.16 |
| (1,2315) | 1:46:A:VAL:HG21 | 1:50:A:LEU:HG | 2 | 0.16 |
| (1,2315) | 1:46:A:VAL:HG22 | 1:50:A:LEU:HG | 2 | 0.16 |
| (1,2315) | 1:46:A:VAL:HG23 | 1:50:A:LEU:HG | 2 | 0.16 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 17 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG11 | 15 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG12 | 15 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG13 | 15 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG21 | 15 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG22 | 15 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HG23 | 15 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG11 | 15 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG12 | 15 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG13 | 15 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG21 | 15 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG22 | 15 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HG23 | 15 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG11 | 15 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG12 | 15 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG13 | 15 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG21 | 15 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG22 | 15 | 0.16 |
| (1,2237) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HG23 | 15 | 0.16 |
| (1,2171) | 1:86:A:LYS:H | 1:87:A:ILE:HG12 | 12 | 0.16 |
| (1,2168) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HG2 | 4 | 0.16 |
| (1,2168) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HG2 | 4 | 0.16 |
| (1,2168) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HG2 | 19 | 0.16 |
| (1,2168) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HG2 | 19 | 0.16 |
| (1,2159) | 1:76:A:ALA:HA | 1:79:A:ILE:HG12 | 20 | 0.16 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 4 | 0.16 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 4 | 0.16 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 18 | 0.16 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 18 | 0.16 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG21 | 3 | 0.16 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG22 | 3 | 0.16 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG23 | 3 | 0.16 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG21 | 3 | 0.16 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG22 | 3 | 0.16 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG23 | 3 | 0.16 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG21 | 16 | 0.16 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG22 | 16 | 0.16 |
| (1,2093) | 1:90:A:PRO:HG2 | 1:110:A:VAL:HG23 | 16 | 0.16 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG21 | 16 | 0.16 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG22 | 16 | 0.16 |
| (1,2093) | 1:90:A:PRO:HG3 | 1:110:A:VAL:HG23 | 16 | 0.16 |
| (1,2072) | 1:93:A:GLU:HA | 1:97:A:LYS:HD2 | 11 | 0.16 |
| (1,2072) | 1:93:A:GLU:HA | 1:97:A:LYS:HD2 | 13 | 0.16 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 11 | 0.16 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 19 | 0.16 |
| (1,1930) | 1:186:A:GLU:HB3 | 1:187:A:LYS:H | 1 | 0.16 |
| (1,1930) | 1:186:A:GLU:HB3 | 1:187:A:LYS:H | 6 | 0.16 |
| (1,1930) | 1:186:A:GLU:HB3 | 1:187:A:LYS:H | 15 | 0.16 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG21 | 4 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG22 | 4 | 0.16 |
| (1,1917) | 1:91:A:MET:HB2 | 1:110:A:VAL:HG23 | 4 | 0.16 |
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 9 | 0.16 |
| (1,1832) | 1:124:A:ALA:HB1 | 1:130:A:VAL:HB | 12 | 0.16 |
| (1,1832) | 1:124:A:ALA:HB2 | 1:130:A:VAL:HB | 12 | 0.16 |
| (1,1832) | 1:124:A:ALA:HB3 | 1:130:A:VAL:HB | 12 | 0.16 |
| (1,1832) | 1:124:A:ALA:HB1 | 1:130:A:VAL:HB | 19 | 0.16 |
| (1,1832) | 1:124:A:ALA:HB2 | 1:130:A:VAL:HB | 19 | 0.16 |
| (1,1832) | 1:124:A:ALA:HB3 | 1:130:A:VAL:HB | 19 | 0.16 |
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 12 | 0.16 |
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 16 | 0.16 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 1 | 0.16 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 8 | 0.16 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 10 | 0.16 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 11 | 0.16 |
| (1,1792) | 1:56:A:MET:HB2 | 1:56:A:MET:HG3 | 1 | 0.16 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 4 | 0.16 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 5 | 0.16 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 8 | 0.16 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 19 | 0.16 |
| (1,1785) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD2 | 15 | 0.16 |
| (1,1701) | 1:136:A:GLN:H | 1:136:A:GLN:HG3 | 7 | 0.16 |
| (1,1696) | 1:48:A:GLN:HA | 1:48:A:GLN:HG3 | 9 | 0.16 |
| (1,1695) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HE22 | 9 | 0.16 |
| (1,1694) | 1:136:A:GLN:HG2 | 1:137:A:GLN:H | 6 | 0.16 |
| (1,1685) | 1:99:A:GLN:HA | 1:99:A:GLN:HG3 | 17 | 0.16 |
| (1,1632) | 1:31:A:PRO:HA | 1:96:A:GLN:HG2 | 5 | 0.16 |
| (1,1547) | 1:152:A:MET:HB3 | 1:160:A:LEU:HD11 | 18 | 0.16 |
| (1,1547) | 1:152:A:MET:HB3 | 1:160:A:LEU:HD12 | 18 | 0.16 |
| (1,1547) | 1:152:A:MET:HB3 | 1:160:A:LEU:HD13 | 18 | 0.16 |
| (1,1474) | 1:161:A:ASN:HB2 | 1:161:A:ASN:HD22 | 2 | 0.16 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG11 | 15 | 0.16 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG12 | 15 | 0.16 |
| (1,1453) | 1:45:A:ASN:HB3 | 1:46:A:VAL:HG13 | 15 | 0.16 |
| (1,1438) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HB2 | 9 | 0.16 |
| (1,1438) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HB2 | 9 | 0.16 |
| (1,1438) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HB2 | 9 | 0.16 |
| (1,1426) | 1:143:A:ASP:HB2 | 1:144:A:LEU:HG | 10 | 0.16 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 4 | 0.16 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 4 | 0.16 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 4 | 0.16 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 8 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 8 | 0.16 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 8 | 0.16 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 18 | 0.16 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 18 | 0.16 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 18 | 0.16 |
| (1,1331) | 1:70:A:ASP:HB3 | 1:72:A:THR:H | 13 | 0.16 |
| (1,1331) | 1:70:A:ASP:HB3 | 1:72:A:THR:H | 17 | 0.16 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 13 | 0.16 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB2 | 4 | 0.16 |
| (1,1318) | 1:23:A:LEU:HG | 1:153:A:TYR:HB3 | 4 | 0.16 |
| (1,1298) | 1:141:A:ALA:HA | 1:146:A:LEU:HB2 | 10 | 0.16 |
| (1,1191) | 1:64:A:LEU:HD11 | 1:65:A:GLY:H | 16 | 0.16 |
| (1,1191) | 1:64:A:LEU:HD12 | 1:65:A:GLY:H | 16 | 0.16 |
| (1,1191) | 1:64:A:LEU:HD13 | 1:65:A:GLY:H | 16 | 0.16 |
| (1,1164) | 1:27:A:SER:H | 1:30:A:CYS:HB3 | 4 | 0.16 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG11 | 12 | 0.16 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG12 | 12 | 0.16 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG13 | 12 | 0.16 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG11 | 20 | 0.16 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG12 | 20 | 0.16 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG13 | 20 | 0.16 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 20 | 0.16 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 20 | 0.16 |
| (1,979) | 1:29:A:TYR:H | 1:71:A:LEU:HD11 | 19 | 0.16 |
| (1,979) | 1:29:A:TYR:H | 1:71:A:LEU:HD12 | 19 | 0.16 |
| (1,979) | 1:29:A:TYR:H | 1:71:A:LEU:HD13 | 19 | 0.16 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 3 | 0.16 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 17 | 0.16 |
| (1,938) | 1:112:A:VAL:HG11 | 1:118:A:GLY:H | 15 | 0.16 |
| (1,938) | 1:112:A:VAL:HG12 | 1:118:A:GLY:H | 15 | 0.16 |
| (1,938) | 1:112:A:VAL:HG13 | 1:118:A:GLY:H | 15 | 0.16 |
| (1,845) | 1:83:A:VAL:HG21 | 1:85:A:ASP:H | 2 | 0.16 |
| (1,845) | 1:83:A:VAL:HG22 | 1:85:A:ASP:H | 2 | 0.16 |
| (1,845) | 1:83:A:VAL:HG23 | 1:85:A:ASP:H | 2 | 0.16 |
| (1,809) | 1:179:A:ASP:HA | 1:180:A:THR:H | 16 | 0.16 |
| (1,797) | 1:46:A:VAL:HA | 1:179:A:ASP:H | 2 | 0.16 |
| (1,683) | 1:168:A:SER:H | 1:170:A:MET:HG2 | 10 | 0.16 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 12 | 0.16 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 9 | 0.16 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 15 | 0.16 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 17 | 0.16 |
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 15 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,599) | 1:183:A:GLN:HB3 | 1:184:A:LEU:H | 10 | 0.16 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 20 | 0.16 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 20 | 0.16 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 20 | 0.16 |
| (1,570) | 1:50:A:LEU:H | 1:51:A:PRO:HD3 | 14 | 0.16 |
| (1,560) | 1:42:A:VAL:HG21 | 1:178:A:ALA:H | 20 | 0.16 |
| (1,560) | 1:42:A:VAL:HG22 | 1:178:A:ALA:H | 20 | 0.16 |
| (1,560) | 1:42:A:VAL:HG23 | 1:178:A:ALA:H | 20 | 0.16 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 10 | 0.16 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 10 | 0.16 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 10 | 0.16 |
| (1,300) | 1:130:A:VAL:HG21 | 1:131:A:LYS:H | 5 | 0.16 |
| (1,300) | 1:130:A:VAL:HG22 | 1:131:A:LYS:H | 5 | 0.16 |
| (1,300) | 1:130:A:VAL:HG23 | 1:131:A:LYS:H | 5 | 0.16 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 5 | 0.16 |
| (1,241) | 1:70:A:ASP:HB2 | 1:74:A:ALA:H | 1 | 0.16 |
| (1,138) | 1:80:A:ALA:H | 1:81:A:LEU:HA | 16 | 0.16 |
| (1,67) | 1:26:A:PHE:H | 1:59:A:TYR:H | 9 | 0.16 |
| (1,40) | 1:5:A:ASP:H | 1:7:A:LYS:HB2 | 6 | 0.16 |
| (1,40) | 1:5:A:ASP:H | 1:7:A:LYS:HB2 | 17 | 0.16 |
| (1,3) | 1:152:A:MET:HB3 | 1:160:A:LEU:H | 18 | 0.16 |
| (1,3521) | 1:162:A:PRO:HG2 | 1:177:A:TYR:HE1 | 15 | 0.15 |
| (1,3521) | 1:162:A:PRO:HG2 | 1:177:A:TYR:HE2 | 15 | 0.15 |
| (1,3521) | 1:162:A:PRO:HG3 | 1:177:A:TYR:HE1 | 15 | 0.15 |
| (1,3521) | 1:162:A:PRO:HG3 | 1:177:A:TYR:HE2 | 15 | 0.15 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE1 | 10 | 0.15 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE2 | 10 | 0.15 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE1 | 10 | 0.15 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE2 | 10 | 0.15 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE1 | 8 | 0.15 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE2 | 8 | 0.15 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE1 | 18 | 0.15 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE2 | 18 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE1 | 2 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE2 | 2 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE1 | 2 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE2 | 2 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE1 | 2 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE2 | 2 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE1 | 11 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE2 | 11 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE1 | 11 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE2 | 11 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE1 | 11 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE2 | 11 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE1 | 16 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE2 | 16 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE1 | 16 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE2 | 16 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE1 | 16 | 0.15 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE2 | 16 | 0.15 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 14 | 0.15 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 14 | 0.15 |
| (1,3463) | 1:77:A:VAL:H | 1:125:A:TRP:HE3 | 17 | 0.15 |
| (1,3463) | 1:77:A:VAL:H | 1:125:A:TRP:HE3 | 20 | 0.15 |
| (1,3461) | 1:75:A:TRP:HB3 | 1:75:A:TRP:HE3 | 13 | 0.15 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 14 | 0.15 |
| (1,3452) | 1:75:A:TRP:HZ3 | 1:78:A:ALA:HB1 | 9 | 0.15 |
| (1,3452) | 1:75:A:TRP:HZ3 | 1:78:A:ALA:HB2 | 9 | 0.15 |
| (1,3452) | 1:75:A:TRP:HZ3 | 1:78:A:ALA:HB3 | 9 | 0.15 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 13 | 0.15 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 15 | 0.15 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG2 | 11 | 0.15 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG3 | 11 | 0.15 |
| (1,3430) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HB3 | 8 | 0.15 |
| (1,3419) | 1:75:A:TRP:HB2 | 1:75:A:TRP:HD1 | 3 | 0.15 |
| (1,3417) | 1:36:A:PHE:HD1 | 1:42:A:VAL:HG11 | 12 | 0.15 |
| (1,3417) | 1:36:A:PHE:HD1 | 1:42:A:VAL:HG12 | 12 | 0.15 |
| (1,3417) | 1:36:A:PHE:HD1 | 1:42:A:VAL:HG13 | 12 | 0.15 |
| (1,3417) | 1:36:A:PHE:HD2 | 1:42:A:VAL:HG11 | 12 | 0.15 |
| (1,3417) | 1:36:A:PHE:HD2 | 1:42:A:VAL:HG12 | 12 | 0.15 |
| (1,3417) | 1:36:A:PHE:HD2 | 1:42:A:VAL:HG13 | 12 | 0.15 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD11 | 16 | 0.15 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD12 | 16 | 0.15 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD13 | 16 | 0.15 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD11 | 16 | 0.15 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD12 | 16 | 0.15 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD13 | 16 | 0.15 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD11 | 18 | 0.15 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD12 | 18 | 0.15 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD13 | 18 | 0.15 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD11 | 18 | 0.15 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD12 | 18 | 0.15 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD13 | 18 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3412) | 1:36:A:PHE:HD1 | 1:40:A:LEU:HD11 | 13 | 0.15 |
| (1,3412) | 1:36:A:PHE:HD1 | 1:40:A:LEU:HD12 | 13 | 0.15 |
| (1,3412) | 1:36:A:PHE:HD1 | 1:40:A:LEU:HD13 | 13 | 0.15 |
| (1,3412) | 1:36:A:PHE:HD2 | 1:40:A:LEU:HD11 | 13 | 0.15 |
| (1,3412) | 1:36:A:PHE:HD2 | 1:40:A:LEU:HD12 | 13 | 0.15 |
| (1,3412) | 1:36:A:PHE:HD2 | 1:40:A:LEU:HD13 | 13 | 0.15 |
| (1,3407) | 1:59:A:TYR:HD1 | 1:60:A:HIS:H | 3 | 0.15 |
| (1,3407) | 1:59:A:TYR:HD2 | 1:60:A:HIS:H | 3 | 0.15 |
| (1,3395) | 1:26:A:PHE:HD1 | 1:59:A:TYR:H | 10 | 0.15 |
| (1,3395) | 1:26:A:PHE:HD2 | 1:59:A:TYR:H | 10 | 0.15 |
| (1,3378) | 1:40:A:LEU:HD11 | 1:173:A:PHE:HD1 | 17 | 0.15 |
| (1,3378) | 1:40:A:LEU:HD11 | 1:173:A:PHE:HD2 | 17 | 0.15 |
| (1,3378) | 1:40:A:LEU:HD12 | 1:173:A:PHE:HD1 | 17 | 0.15 |
| (1,3378) | 1:40:A:LEU:HD12 | 1:173:A:PHE:HD2 | 17 | 0.15 |
| (1,3378) | 1:40:A:LEU:HD13 | 1:173:A:PHE:HD1 | 17 | 0.15 |
| (1,3378) | 1:40:A:LEU:HD13 | 1:173:A:PHE:HD2 | 17 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD1 | 10 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD2 | 10 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD1 | 10 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD2 | 10 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD1 | 10 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD2 | 10 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD1 | 14 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD2 | 14 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD1 | 14 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD2 | 14 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD1 | 14 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD2 | 14 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD1 | 16 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD2 | 16 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD1 | 16 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD2 | 16 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD1 | 16 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD2 | 16 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD1 | 19 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD2 | 19 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD1 | 19 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD2 | 19 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD1 | 19 | 0.15 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD2 | 19 | 0.15 |
| (1,3356) | 1:25:A:PHE:H | 1:25:A:PHE:HD1 | 2 | 0.15 |
| (1,3356) | 1:25:A:PHE:H | 1:25:A:PHE:HD2 | 2 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3336) | 1:92:A:PHE:HD1 | 1:96:A:GLN:HG2 | 1 | 0.15 |
| (1,3336) | 1:92:A:PHE:HD2 | 1:96:A:GLN:HG2 | 1 | 0.15 |
| (1,3336) | 1:92:A:PHE:HD1 | 1:96:A:GLN:HG2 | 20 | 0.15 |
| (1,3336) | 1:92:A:PHE:HD2 | 1:96:A:GLN:HG2 | 20 | 0.15 |
| (1,3331) | 1:91:A:MET:H | 1:92:A:PHE:HD1 | 13 | 0.15 |
| (1,3331) | 1:91:A:MET:H | 1:92:A:PHE:HD2 | 13 | 0.15 |
| (1,3325) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HD1 | 8 | 0.15 |
| (1,3325) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HD2 | 8 | 0.15 |
| (1,3325) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HD1 | 8 | 0.15 |
| (1,3325) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HD2 | 8 | 0.15 |
| (1,3325) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HD1 | 8 | 0.15 |
| (1,3325) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HD2 | 8 | 0.15 |
| (1,3305) | 1:38:A:GLU:H | 1:41:A:HIS:HE1 | 1 | 0.15 |
| (1,3305) | 1:38:A:GLU:H | 1:41:A:HIS:HE1 | 3 | 0.15 |
| (1,3305) | 1:38:A:GLU:H | 1:41:A:HIS:HE1 | 5 | 0.15 |
| (1,3305) | 1:38:A:GLU:H | 1:41:A:HIS:HE1 | 13 | 0.15 |
| (1,3272) | 1:117:A:LYS:HB2 | 1:118:A:GLY:HA2 | 13 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 1 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 1 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 1 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 1 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 1 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 1 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 15 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 15 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 15 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 15 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 15 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 15 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 17 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 17 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 17 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 17 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 17 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 17 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 19 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 19 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 19 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 19 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 19 | 0.15 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 19 | 0.15 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 15 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 15 | 0.15 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 15 | 0.15 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 15 | 0.15 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 15 | 0.15 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 15 | 0.15 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 15 | 0.15 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 15 | 0.15 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 15 | 0.15 |
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 13 | 0.15 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG11 | 8 | 0.15 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG12 | 8 | 0.15 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG13 | 8 | 0.15 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG11 | 14 | 0.15 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG12 | 14 | 0.15 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG13 | 14 | 0.15 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 1 | 0.15 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 3 | 0.15 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 5 | 0.15 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 12 | 0.15 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 13 | 0.15 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 14 | 0.15 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 15 | 0.15 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 20 | 0.15 |
| (1,2832) | 1:55:A:LYS:HA | 1:56:A:MET:HB2 | 3 | 0.15 |
| (1,2766) | 1:39:A:VAL:HG21 | 1:40:A:LEU:H | 13 | 0.15 |
| (1,2766) | 1:39:A:VAL:HG22 | 1:40:A:LEU:H | 13 | 0.15 |
| (1,2766) | 1:39:A:VAL:HG23 | 1:40:A:LEU:H | 13 | 0.15 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG11 | 1 | 0.15 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG12 | 1 | 0.15 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG13 | 1 | 0.15 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG21 | 12 | 0.15 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG22 | 12 | 0.15 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG23 | 12 | 0.15 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG21 | 18 | 0.15 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG22 | 18 | 0.15 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG23 | 18 | 0.15 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 18 | 0.15 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 18 | 0.15 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 18 | 0.15 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD2 | 11 | 0.15 |
| (1,2614) | 1:11:A:THR:HG21 | 1:157:A:LYS:HD3 | 11 | 0.15 |
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD2 | 11 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2614) | 1:11:A:THR:HG22 | 1:157:A:LYS:HD3 | 11 | 0.15 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD2 | 11 | 0.15 |
| (1,2614) | 1:11:A:THR:HG23 | 1:157:A:LYS:HD3 | 11 | 0.15 |
| (1,2577) | 1:46:A:VAL:HG21 | 1:181:A:VAL:HA | 10 | 0.15 |
| (1,2577) | 1:46:A:VAL:HG22 | 1:181:A:VAL:HA | 10 | 0.15 |
| (1,2577) | 1:46:A:VAL:HG23 | 1:181:A:VAL:HA | 10 | 0.15 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 6 | 0.15 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 6 | 0.15 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 6 | 0.15 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 6 | 0.15 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 6 | 0.15 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 6 | 0.15 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 6 | 0.15 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 6 | 0.15 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 6 | 0.15 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 6 | 0.15 |
| (1,2499) | 1:6:A:GLY:HA3 | 1:10:A:ILE:HA | 10 | 0.15 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 16 | 0.15 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 16 | 0.15 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 16 | 0.15 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 16 | 0.15 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 16 | 0.15 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 16 | 0.15 |
| (1,2417) | 1:73:A:GLN:HA | 1:77:A:VAL:HG21 | 13 | 0.15 |
| (1,2417) | 1:73:A:GLN:HA | 1:77:A:VAL:HG22 | 13 | 0.15 |
| (1,2417) | 1:73:A:GLN:HA | 1:77:A:VAL:HG23 | 13 | 0.15 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 18 | 0.15 |
| (1,2344) | 1:7:A:LYS:HG3 | 1:8:A:GLN:HA | 10 | 0.15 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 2 | 0.15 |
| (1,2233) | 1:25:A:PHE:HB2 | 1:149:A:VAL:HG11 | 3 | 0.15 |
| (1,2233) | 1:25:A:PHE:HB2 | 1:149:A:VAL:HG12 | 3 | 0.15 |
| (1,2233) | 1:25:A:PHE:HB2 | 1:149:A:VAL:HG13 | 3 | 0.15 |
| (1,2233) | 1:25:A:PHE:HB2 | 1:149:A:VAL:HG21 | 3 | 0.15 |
| (1,2233) | 1:25:A:PHE:HB2 | 1:149:A:VAL:HG22 | 3 | 0.15 |
| (1,2233) | 1:25:A:PHE:HB2 | 1:149:A:VAL:HG23 | 3 | 0.15 |
| (1,2233) | 1:25:A:PHE:HB3 | 1:149:A:VAL:HG11 | 3 | 0.15 |
| (1,2233) | 1:25:A:PHE:HB3 | 1:149:A:VAL:HG12 | 3 | 0.15 |
| (1,2233) | 1:25:A:PHE:HB3 | 1:149:A:VAL:HG13 | 3 | 0.15 |
| (1,2233) | 1:25:A:PHE:HB3 | 1:149:A:VAL:HG21 | 3 | 0.15 |
| (1,2233) | 1:25:A:PHE:HB3 | 1:149:A:VAL:HG22 | 3 | 0.15 |
| (1,2233) | 1:25:A:PHE:HB3 | 1:149:A:VAL:HG23 | 3 | 0.15 |
| (1,2171) | 1:86:A:LYS:H | 1:87:A:ILE:HG12 | 9 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2168) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HG2 | 13 | 0.15 |
| (1,2168) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HG2 | 13 | 0.15 |
| (1,2118) | 1:10:A:ILE:HG13 | 1:159:A:GLN:H | 14 | 0.15 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG11 | 9 | 0.15 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG12 | 9 | 0.15 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG13 | 9 | 0.15 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 10 | 0.15 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 19 | 0.15 |
| (1,2015) | 1:117:A:LYS:HB2 | 1:117:A:LYS:HD3 | 3 | 0.15 |
| (1,2015) | 1:117:A:LYS:HB2 | 1:117:A:LYS:HD3 | 4 | 0.15 |
| (1,1989) | 1:136:A:GLN:HB2 | 1:137:A:GLN:H | 2 | 0.15 |
| (1,1930) | 1:186:A:GLU:HB3 | 1:187:A:LYS:H | 2 | 0.15 |
| (1,1930) | 1:186:A:GLU:HB3 | 1:187:A:LYS:H | 20 | 0.15 |
| (1,1902) | 1:147:A:GLN:HB3 | 1:148:A:GLY:HA2 | 6 | 0.15 |
| (1,1848) | 1:83:A:VAL:HB | 1:87:A:ILE:HG13 | 13 | 0.15 |
| (1,1832) | 1:124:A:ALA:HB1 | 1:130:A:VAL:HB | 8 | 0.15 |
| (1,1832) | 1:124:A:ALA:HB2 | 1:130:A:VAL:HB | 8 | 0.15 |
| (1,1832) | 1:124:A:ALA:HB3 | 1:130:A:VAL:HB | 8 | 0.15 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 4 | 0.15 |
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 14 | 0.15 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE1 | 17 | 0.15 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE2 | 17 | 0.15 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE3 | 17 | 0.15 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE1 | 19 | 0.15 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE2 | 19 | 0.15 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE3 | 19 | 0.15 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 3 | 0.15 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 6 | 0.15 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 19 | 0.15 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 1 | 0.15 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 9 | 0.15 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 12 | 0.15 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 16 | 0.15 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 17 | 0.15 |
| (1,1785) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD2 | 17 | 0.15 |
| (1,1758) | 1:14:A:LYS:H | 1:14:A:LYS:HB3 | 15 | 0.15 |
| (1,1699) | 1:135:A:ALA:HB1 | 1:136:A:GLN:HG2 | 14 | 0.15 |
| (1,1699) | 1:135:A:ALA:HB2 | 1:136:A:GLN:HG2 | 14 | 0.15 |
| (1,1699) | 1:135:A:ALA:HB3 | 1:136:A:GLN:HG2 | 14 | 0.15 |
| (1,1695) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HE22 | 7 | 0.15 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG2 | 20 | 0.15 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG3 | 20 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1536) | 1:154:A:VAL:HG21 | 1:155:A:ASN:HB2 | 7 | 0.15 |
| (1,1536) | 1:154:A:VAL:HG22 | 1:155:A:ASN:HB2 | 7 | 0.15 |
| (1,1536) | 1:154:A:VAL:HG23 | 1:155:A:ASN:HB2 | 7 | 0.15 |
| (1,1474) | 1:161:A:ASN:HB2 | 1:161:A:ASN:HD22 | 3 | 0.15 |
| (1,1474) | 1:161:A:ASN:HB2 | 1:161:A:ASN:HD22 | 4 | 0.15 |
| (1,1474) | 1:161:A:ASN:HB2 | 1:161:A:ASN:HD22 | 13 | 0.15 |
| (1,1450) | 1:42:A:VAL:HA | 1:45:A:ASN:HB3 | 3 | 0.15 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB2 | 20 | 0.15 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB3 | 20 | 0.15 |
| (1,1294) | 1:71:A:LEU:HB2 | 1:74:A:ALA:H | 17 | 0.15 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG11 | 3 | 0.15 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG12 | 3 | 0.15 |
| (1,1159) | 1:149:A:VAL:H | 1:149:A:VAL:HG13 | 3 | 0.15 |
| (1,1116) | 1:61:A:VAL:HG11 | 1:63:A:PHE:H | 20 | 0.15 |
| (1,1116) | 1:61:A:VAL:HG12 | 1:63:A:PHE:H | 20 | 0.15 |
| (1,1116) | 1:61:A:VAL:HG13 | 1:63:A:PHE:H | 20 | 0.15 |
| (1,1080) | 1:34:A:TYR:HD2 | 1:38:A:GLU:H | 11 | 0.15 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 1 | 0.15 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 6 | 0.15 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 11 | 0.15 |
| (1,1005) | 1:46:A:VAL:HG21 | 1:48:A:GLN:H | 10 | 0.15 |
| (1,1005) | 1:46:A:VAL:HG22 | 1:48:A:GLN:H | 10 | 0.15 |
| (1,1005) | 1:46:A:VAL:HG23 | 1:48:A:GLN:H | 10 | 0.15 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 10 | 0.15 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 15 | 0.15 |
| (1,975) | 1:99:A:GLN:H | 1:99:A:GLN:HB3 | 13 | 0.15 |
| (1,938) | 1:112:A:VAL:HG11 | 1:118:A:GLY:H | 10 | 0.15 |
| (1,938) | 1:112:A:VAL:HG12 | 1:118:A:GLY:H | 10 | 0.15 |
| (1,938) | 1:112:A:VAL:HG13 | 1:118:A:GLY:H | 10 | 0.15 |
| (1,919) | 1:37:A:GLU:H | 1:38:A:GLU:HB3 | 12 | 0.15 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 2 | 0.15 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD21 | 7 | 0.15 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD22 | 7 | 0.15 |
| (1,808) | 1:158:A:TYR:H | 1:184:A:LEU:HD23 | 7 | 0.15 |
| (1,756) | 1:79:A:ILE:H | 1:79:A:ILE:HG12 | 8 | 0.15 |
| (1,650) | 1:145:A:GLN:HA | 1:146:A:LEU:H | 5 | 0.15 |
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 7 | 0.15 |
| (1,639) | 1:12:A:LEU:HB2 | 1:14:A:LYS:H | 17 | 0.15 |
| (1,632) | 1:87:A:ILE:HG21 | 1:91:A:MET:H | 5 | 0.15 |
| (1,632) | 1:87:A:ILE:HG22 | 1:91:A:MET:H | 5 | 0.15 |
| (1,632) | 1:87:A:ILE:HG23 | 1:91:A:MET:H | 5 | 0.15 |
| (1,632) | 1:87:A:ILE:HG21 | 1:91:A:MET:H | 8 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,632) | 1:87:A:ILE:HG22 | 1:91:A:MET:H | 8 | 0.15 |
| (1,632) | 1:87:A:ILE:HG23 | 1:91:A:MET:H | 8 | 0.15 |
| (1,632) | 1:87:A:ILE:HG21 | 1:91:A:MET:H | 9 | 0.15 |
| (1,632) | 1:87:A:ILE:HG22 | 1:91:A:MET:H | 9 | 0.15 |
| (1,632) | 1:87:A:ILE:HG23 | 1:91:A:MET:H | 9 | 0.15 |
| (1,632) | 1:87:A:ILE:HG21 | 1:91:A:MET:H | 12 | 0.15 |
| (1,632) | 1:87:A:ILE:HG22 | 1:91:A:MET:H | 12 | 0.15 |
| (1,632) | 1:87:A:ILE:HG23 | 1:91:A:MET:H | 12 | 0.15 |
| (1,599) | 1:183:A:GLN:HB3 | 1:184:A:LEU:H | 18 | 0.15 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 5 | 0.15 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 5 | 0.15 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 5 | 0.15 |
| (1,587) | 1:46:A:VAL:HG21 | 1:47:A:ARG:H | 8 | 0.15 |
| (1,587) | 1:46:A:VAL:HG22 | 1:47:A:ARG:H | 8 | 0.15 |
| (1,587) | 1:46:A:VAL:HG23 | 1:47:A:ARG:H | 8 | 0.15 |
| (1,555) | 1:174:A:VAL:HG21 | 1:178:A:ALA:H | 12 | 0.15 |
| (1,555) | 1:174:A:VAL:HG22 | 1:178:A:ALA:H | 12 | 0.15 |
| (1,555) | 1:174:A:VAL:HG23 | 1:178:A:ALA:H | 12 | 0.15 |
| (1,441) | 1:34:A:TYR:HE2 | 1:92:A:PHE:H | 1 | 0.15 |
| (1,337) | 1:166:A:ASP:H | 1:176:A:GLN:HE21 | 11 | 0.15 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 6 | 0.15 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 6 | 0.15 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 6 | 0.15 |
| (1,300) | 1:130:A:VAL:HG21 | 1:131:A:LYS:H | 13 | 0.15 |
| (1,300) | 1:130:A:VAL:HG22 | 1:131:A:LYS:H | 13 | 0.15 |
| (1,300) | 1:130:A:VAL:HG23 | 1:131:A:LYS:H | 13 | 0.15 |
| (1,300) | 1:130:A:VAL:HG21 | 1:131:A:LYS:H | 19 | 0.15 |
| (1,300) | 1:130:A:VAL:HG22 | 1:131:A:LYS:H | 19 | 0.15 |
| (1,300) | 1:130:A:VAL:HG23 | 1:131:A:LYS:H | 19 | 0.15 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 19 | 0.15 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 20 | 0.15 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 16 | 0.15 |
| (1,216) | 1:34:A:TYR:H | 1:96:A:GLN:HE21 | 2 | 0.15 |
| (1,216) | 1:34:A:TYR:H | 1:96:A:GLN:HE21 | 11 | 0.15 |
| (1,165) | 1:67:A:LEU:H | 1:69:A:LYS:H | 9 | 0.15 |
| (1,159) | 1:62:A:GLU:HG3 | 1:69:A:LYS:H | 10 | 0.15 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD21 | 13 | 0.15 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD22 | 13 | 0.15 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD23 | 13 | 0.15 |
| (1,138) | 1:80:A:ALA:H | 1:81:A:LEU:HA | 2 | 0.15 |
| (1,138) | 1:80:A:ALA:H | 1:81:A:LEU:HA | 3 | 0.15 |
| (1,138) | 1:80:A:ALA:H | 1:81:A:LEU:HA | 4 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,138) | 1:80:A:ALA:H | 1:81:A:LEU:HA | 12 | 0.15 |
| (1,138) | 1:80:A:ALA:H | 1:81:A:LEU:HA | 20 | 0.15 |
| (1,62) | 1:102:A:GLN:H | 1:102:A:GLN:HG2 | 8 | 0.15 |
| (1,62) | 1:102:A:GLN:H | 1:102:A:GLN:HG2 | 10 | 0.15 |
| (1,62) | 1:102:A:GLN:H | 1:102:A:GLN:HG2 | 16 | 0.15 |
| (1,62) | 1:102:A:GLN:H | 1:102:A:GLN:HG2 | 17 | 0.15 |
| (1,62) | 1:102:A:GLN:H | 1:102:A:GLN:HG2 | 19 | 0.15 |
| (1,62) | 1:102:A:GLN:H | 1:102:A:GLN:HG2 | 20 | 0.15 |
| (1,3531) | 1:58:A:LYS:H | 1:75:A:TRP:HZ2 | 11 | 0.14 |
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 8 | 0.14 |
| (1,3523) | 1:73:A:GLN:HE21 | 1:125:A:TRP:HZ2 | 1 | 0.14 |
| (1,3523) | 1:73:A:GLN:HE21 | 1:125:A:TRP:HZ2 | 15 | 0.14 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE1 | 9 | 0.14 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE2 | 9 | 0.14 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE1 | 14 | 0.14 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE2 | 14 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 3 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 3 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 6 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 6 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 9 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 9 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 15 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 15 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 16 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 16 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 18 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 18 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 19 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 19 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 20 | 0.14 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 20 | 0.14 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE1 | 4 | 0.14 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE2 | 4 | 0.14 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE1 | 4 | 0.14 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE2 | 4 | 0.14 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE1 | 18 | 0.14 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE2 | 18 | 0.14 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE1 | 18 | 0.14 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE2 | 18 | 0.14 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE1 | 6 | 0.14 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE2 | 6 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE1 | 17 | 0.14 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE2 | 17 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE1 | 6 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE2 | 6 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE1 | 6 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE2 | 6 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE1 | 6 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE2 | 6 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE1 | 14 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE2 | 14 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE1 | 14 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE2 | 14 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE1 | 14 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE2 | 14 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE1 | 15 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE2 | 15 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE1 | 15 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE2 | 15 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE1 | 15 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE2 | 15 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE1 | 17 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE2 | 17 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE1 | 17 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE2 | 17 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE1 | 17 | 0.14 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE2 | 17 | 0.14 |
| (1,3463) | 1:77:A:VAL:H | 1:125:A:TRP:HE3 | 5 | 0.14 |
| (1,3463) | 1:77:A:VAL:H | 1:125:A:TRP:HE3 | 10 | 0.14 |
| (1,3463) | 1:77:A:VAL:H | 1:125:A:TRP:HE3 | 11 | 0.14 |
| (1,3463) | 1:77:A:VAL:H | 1:125:A:TRP:HE3 | 19 | 0.14 |
| (1,3461) | 1:75:A:TRP:HB3 | 1:75:A:TRP:HE3 | 8 | 0.14 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 1 | 0.14 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 2 | 0.14 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 3 | 0.14 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 5 | 0.14 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 13 | 0.14 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 19 | 0.14 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 2 | 0.14 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 4 | 0.14 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 6 | 0.14 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 9 | 0.14 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 10 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 11 | 0.14 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 12 | 0.14 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 16 | 0.14 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 17 | 0.14 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 20 | 0.14 |
| (1,3438) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HH2 | 8 | 0.14 |
| (1,3422) | 1:60:A:HIS:H | 1:75:A:TRP:HD1 | 13 | 0.14 |
| (1,3422) | 1:60:A:HIS:H | 1:75:A:TRP:HD1 | 15 | 0.14 |
| (1,3419) | 1:75:A:TRP:HB2 | 1:75:A:TRP:HD1 | 19 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD11 | 7 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD12 | 7 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD13 | 7 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD11 | 7 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD12 | 7 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD13 | 7 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD11 | 8 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD12 | 8 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD13 | 8 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD11 | 8 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD12 | 8 | 0.14 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD13 | 8 | 0.14 |
| (1,3414) | 1:59:A:TYR:HD1 | 1:137:A:GLN:HB2 | 10 | 0.14 |
| (1,3414) | 1:59:A:TYR:HD1 | 1:137:A:GLN:HB3 | 10 | 0.14 |
| (1,3414) | 1:59:A:TYR:HD2 | 1:137:A:GLN:HB2 | 10 | 0.14 |
| (1,3414) | 1:59:A:TYR:HD2 | 1:137:A:GLN:HB3 | 10 | 0.14 |
| (1,3407) | 1:59:A:TYR:HD1 | 1:60:A:HIS:H | 5 | 0.14 |
| (1,3407) | 1:59:A:TYR:HD2 | 1:60:A:HIS:H | 5 | 0.14 |
| (1,3407) | 1:59:A:TYR:HD1 | 1:60:A:HIS:H | 6 | 0.14 |
| (1,3407) | 1:59:A:TYR:HD2 | 1:60:A:HIS:H | 6 | 0.14 |
| (1,3404) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HB2 | 5 | 0.14 |
| (1,3404) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HB3 | 5 | 0.14 |
| (1,3404) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HB2 | 5 | 0.14 |
| (1,3404) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HB3 | 5 | 0.14 |
| (1,3404) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HB2 | 20 | 0.14 |
| (1,3404) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HB3 | 20 | 0.14 |
| (1,3404) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HB2 | 20 | 0.14 |
| (1,3404) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HB3 | 20 | 0.14 |
| (1,3398) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HG2 | 6 | 0.14 |
| (1,3398) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HG3 | 6 | 0.14 |
| (1,3398) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HG2 | 6 | 0.14 |
| (1,3398) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HG3 | 6 | 0.14 |
| (1,3398) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HG2 | 12 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3398) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HG3 | 12 | 0.14 |
| (1,3398) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HG2 | 12 | 0.14 |
| (1,3398) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HG3 | 12 | 0.14 |
| (1,3396) | 1:25:A:PHE:HA | 1:26:A:PHE:HD1 | 1 | 0.14 |
| (1,3396) | 1:25:A:PHE:HA | 1:26:A:PHE:HD2 | 1 | 0.14 |
| (1,3392) | 1:128:A:PHE:HA | 1:128:A:PHE:HD2 | 3 | 0.14 |
| (1,3392) | 1:128:A:PHE:HA | 1:128:A:PHE:HD2 | 5 | 0.14 |
| (1,3388) | 1:34:A:TYR:HD1 | 1:92:A:PHE:HA | 14 | 0.14 |
| (1,3388) | 1:34:A:TYR:HD2 | 1:92:A:PHE:HA | 14 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD1 | 3 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD2 | 3 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD1 | 3 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD2 | 3 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD1 | 3 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD2 | 3 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD1 | 9 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD2 | 9 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD1 | 9 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD2 | 9 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD1 | 9 | 0.14 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD2 | 9 | 0.14 |
| (1,3371) | 1:167:A:THR:HG21 | 1:173:A:PHE:HD1 | 15 | 0.14 |
| (1,3371) | 1:167:A:THR:HG21 | 1:173:A:PHE:HD2 | 15 | 0.14 |
| (1,3371) | 1:167:A:THR:HG22 | 1:173:A:PHE:HD1 | 15 | 0.14 |
| (1,3371) | 1:167:A:THR:HG22 | 1:173:A:PHE:HD2 | 15 | 0.14 |
| (1,3371) | 1:167:A:THR:HG23 | 1:173:A:PHE:HD1 | 15 | 0.14 |
| (1,3371) | 1:167:A:THR:HG23 | 1:173:A:PHE:HD2 | 15 | 0.14 |
| (1,3356) | 1:25:A:PHE:H | 1:25:A:PHE:HD1 | 12 | 0.14 |
| (1,3356) | 1:25:A:PHE:H | 1:25:A:PHE:HD2 | 12 | 0.14 |
| (1,3311) | 1:29:A:TYR:HD1 | 1:71:A:LEU:HB2 | 12 | 0.14 |
| (1,3311) | 1:29:A:TYR:HD2 | 1:71:A:LEU:HB2 | 12 | 0.14 |
| (1,3274) | 1:118:A:GLY:HA3 | 1:121:A:TYR:H | 19 | 0.14 |
| (1,3269) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA2 | 1 | 0.14 |
| (1,3269) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA2 | 1 | 0.14 |
| (1,3269) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA2 | 1 | 0.14 |
| (1,3252) | 1:29:A:TYR:HD1 | 1:68:A:GLY:HA3 | 8 | 0.14 |
| (1,3252) | 1:29:A:TYR:HD2 | 1:68:A:GLY:HA3 | 8 | 0.14 |
| (1,3212) | 1:87:A:ILE:HD11 | 1:91:A:MET:HG2 | 13 | 0.14 |
| (1,3212) | 1:87:A:ILE:HD11 | 1:91:A:MET:HG3 | 13 | 0.14 |
| (1,3212) | 1:87:A:ILE:HD12 | 1:91:A:MET:HG2 | 13 | 0.14 |
| (1,3212) | 1:87:A:ILE:HD12 | 1:91:A:MET:HG3 | 13 | 0.14 |
| (1,3212) | 1:87:A:ILE:HD13 | 1:91:A:MET:HG2 | 13 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3212) | 1:87:A:ILE:HD13 | 1:91:A:MET:HG3 | 13 | 0.14 |
| (1,3212) | 1:87:A:ILE:HD11 | 1:91:A:MET:HG2 | 20 | 0.14 |
| (1,3212) | 1:87:A:ILE:HD11 | 1:91:A:MET:HG3 | 20 | 0.14 |
| (1,3212) | 1:87:A:ILE:HD12 | 1:91:A:MET:HG2 | 20 | 0.14 |
| (1,3212) | 1:87:A:ILE:HD12 | 1:91:A:MET:HG3 | 20 | 0.14 |
| (1,3212) | 1:87:A:ILE:HD13 | 1:91:A:MET:HG2 | 20 | 0.14 |
| (1,3212) | 1:87:A:ILE:HD13 | 1:91:A:MET:HG3 | 20 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 3 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 3 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 3 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 3 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 3 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 3 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 4 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 4 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 4 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 4 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 4 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 4 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 8 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 8 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 8 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 8 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 8 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 8 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 9 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 9 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 9 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 9 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 9 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 9 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 10 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 10 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 10 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 10 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 10 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 10 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 11 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 11 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 11 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 11 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 11 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 11 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 12 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 12 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 12 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 12 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 12 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 12 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 13 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 13 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 13 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 13 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 13 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 13 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 14 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 14 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 14 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 14 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 14 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 14 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 16 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 16 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 16 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 16 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 16 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 16 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 20 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 20 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 20 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 20 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 20 | 0.14 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 20 | 0.14 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG21 | 18 | 0.14 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG22 | 18 | 0.14 |
| (1,3134) | 1:152:A:MET:HE1 | 1:181:A:VAL:HG23 | 18 | 0.14 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG21 | 18 | 0.14 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG22 | 18 | 0.14 |
| (1,3134) | 1:152:A:MET:HE2 | 1:181:A:VAL:HG23 | 18 | 0.14 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG21 | 18 | 0.14 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG22 | 18 | 0.14 |
| (1,3134) | 1:152:A:MET:HE3 | 1:181:A:VAL:HG23 | 18 | 0.14 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD1 | 8 | 0.14 |
| (1,3129) | 1:152:A:MET:HE1 | 1:177:A:TYR:HD2 | 8 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD1 | 8 | 0.14 |
| (1,3129) | 1:152:A:MET:HE2 | 1:177:A:TYR:HD2 | 8 | 0.14 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD1 | 8 | 0.14 |
| (1,3129) | 1:152:A:MET:HE3 | 1:177:A:TYR:HD2 | 8 | 0.14 |
| (1,2943) | 1:3:A:ILE:HG21 | 1:8:A:GLN:HG3 | 15 | 0.14 |
| (1,2943) | 1:3:A:ILE:HG22 | 1:8:A:GLN:HG3 | 15 | 0.14 |
| (1,2943) | 1:3:A:ILE:HG23 | 1:8:A:GLN:HG3 | 15 | 0.14 |
| (1,2935) | 1:75:A:TRP:HA | 1:78:A:ALA:HA | 4 | 0.14 |
| (1,2908) | 1:175:A:ALA:HA | 1:178:A:ALA:H | 16 | 0.14 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 2 | 0.14 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 4 | 0.14 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 9 | 0.14 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 18 | 0.14 |
| (1,2847) | 1:2:A:GLN:HA | 1:2:A:GLN:HB3 | 18 | 0.14 |
| (1,2787) | 1:86:A:LYS:H | 1:87:A:ILE:HG21 | 1 | 0.14 |
| (1,2787) | 1:86:A:LYS:H | 1:87:A:ILE:HG22 | 1 | 0.14 |
| (1,2787) | 1:86:A:LYS:H | 1:87:A:ILE:HG23 | 1 | 0.14 |
| (1,2787) | 1:86:A:LYS:H | 1:87:A:ILE:HG21 | 6 | 0.14 |
| (1,2787) | 1:86:A:LYS:H | 1:87:A:ILE:HG22 | 6 | 0.14 |
| (1,2787) | 1:86:A:LYS:H | 1:87:A:ILE:HG23 | 6 | 0.14 |
| (1,2755) | 1:62:A:GLU:HA | 1:68:A:GLY:HA2 | 13 | 0.14 |
| (1,2748) | 1:7:A:LYS:HA | 1:10:A:ILE:HD11 | 18 | 0.14 |
| (1,2748) | 1:7:A:LYS:HA | 1:10:A:ILE:HD12 | 18 | 0.14 |
| (1,2748) | 1:7:A:LYS:HA | 1:10:A:ILE:HD13 | 18 | 0.14 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG11 | 10 | 0.14 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG12 | 10 | 0.14 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG13 | 10 | 0.14 |
| (1,2724) | 1:124:A:ALA:HA | 1:130:A:VAL:HG11 | 17 | 0.14 |
| (1,2724) | 1:124:A:ALA:HA | 1:130:A:VAL:HG12 | 17 | 0.14 |
| (1,2724) | 1:124:A:ALA:HA | 1:130:A:VAL:HG13 | 17 | 0.14 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG21 | 15 | 0.14 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG22 | 15 | 0.14 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG23 | 15 | 0.14 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG21 | 15 | 0.14 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG22 | 15 | 0.14 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG23 | 15 | 0.14 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG21 | 15 | 0.14 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG22 | 15 | 0.14 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG23 | 15 | 0.14 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG21 | 1 | 0.14 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG22 | 1 | 0.14 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG23 | 1 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG21 | 6 | 0.14 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG22 | 6 | 0.14 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG23 | 6 | 0.14 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG21 | 8 | 0.14 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG22 | 8 | 0.14 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG23 | 8 | 0.14 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG21 | 10 | 0.14 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG22 | 10 | 0.14 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG23 | 10 | 0.14 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG21 | 16 | 0.14 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG22 | 16 | 0.14 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG23 | 16 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD11 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD12 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD13 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD21 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD22 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD23 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD11 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD12 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD13 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD21 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD22 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD23 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD11 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD12 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD13 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD21 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD22 | 13 | 0.14 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD23 | 13 | 0.14 |
| (1,2657) | 1:167:A:THR:HA | 1:167:A:THR:HG21 | 1 | 0.14 |
| (1,2657) | 1:167:A:THR:HA | 1:167:A:THR:HG22 | 1 | 0.14 |
| (1,2657) | 1:167:A:THR:HA | 1:167:A:THR:HG23 | 1 | 0.14 |
| (1,2657) | 1:167:A:THR:HA | 1:167:A:THR:HG21 | 15 | 0.14 |
| (1,2657) | 1:167:A:THR:HA | 1:167:A:THR:HG22 | 15 | 0.14 |
| (1,2657) | 1:167:A:THR:HA | 1:167:A:THR:HG23 | 15 | 0.14 |
| (1,2632) | 1:101:A:VAL:HG21 | 1:107:A:ILE:H | 11 | 0.14 |
| (1,2632) | 1:101:A:VAL:HG22 | 1:107:A:ILE:H | 11 | 0.14 |
| (1,2632) | 1:101:A:VAL:HG23 | 1:107:A:ILE:H | 11 | 0.14 |
| (1,2632) | 1:101:A:VAL:HG21 | 1:107:A:ILE:H | 15 | 0.14 |
| (1,2632) | 1:101:A:VAL:HG22 | 1:107:A:ILE:H | 15 | 0.14 |
| (1,2632) | 1:101:A:VAL:HG23 | 1:107:A:ILE:H | 15 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2630) | 1:101:A:VAL:HG21 | 1:102:A:GLN:H | 9 | 0.14 |
| (1,2630) | 1:101:A:VAL:HG22 | 1:102:A:GLN:H | 9 | 0.14 |
| (1,2630) | 1:101:A:VAL:HG23 | 1:102:A:GLN:H | 9 | 0.14 |
| (1,2630) | 1:101:A:VAL:HG21 | 1:102:A:GLN:H | 18 | 0.14 |
| (1,2630) | 1:101:A:VAL:HG22 | 1:102:A:GLN:H | 18 | 0.14 |
| (1,2630) | 1:101:A:VAL:HG23 | 1:102:A:GLN:H | 18 | 0.14 |
| (1,2621) | 1:101:A:VAL:HG21 | 1:106:A:ASP:H | 11 | 0.14 |
| (1,2621) | 1:101:A:VAL:HG22 | 1:106:A:ASP:H | 11 | 0.14 |
| (1,2621) | 1:101:A:VAL:HG23 | 1:106:A:ASP:H | 11 | 0.14 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 16 | 0.14 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 16 | 0.14 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 16 | 0.14 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 16 | 0.14 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 16 | 0.14 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 16 | 0.14 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 16 | 0.14 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 16 | 0.14 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 16 | 0.14 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG21 | 11 | 0.14 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG22 | 11 | 0.14 |
| (1,2572) | 1:51:A:PRO:HD3 | 1:54:A:THR:HG23 | 11 | 0.14 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD21 | 2 | 0.14 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD22 | 2 | 0.14 |
| (1,2550) | 1:154:A:VAL:HG21 | 1:184:A:LEU:HD23 | 2 | 0.14 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD21 | 2 | 0.14 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD22 | 2 | 0.14 |
| (1,2550) | 1:154:A:VAL:HG22 | 1:184:A:LEU:HD23 | 2 | 0.14 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD21 | 2 | 0.14 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD22 | 2 | 0.14 |
| (1,2550) | 1:154:A:VAL:HG23 | 1:184:A:LEU:HD23 | 2 | 0.14 |
| (1,2529) | 1:97:A:LYS:H | 1:98:A:THR:HG21 | 4 | 0.14 |
| (1,2529) | 1:97:A:LYS:H | 1:98:A:THR:HG22 | 4 | 0.14 |
| (1,2529) | 1:97:A:LYS:H | 1:98:A:THR:HG23 | 4 | 0.14 |
| (1,2484) | 1:183:A:GLN:HA | 1:183:A:GLN:HB2 | 15 | 0.14 |
| (1,2435) | 1:131:A:LYS:HA | 1:134:A:VAL:HA | 10 | 0.14 |
| (1,2334) | 1:3:A:ILE:HA | 1:8:A:GLN:HG3 | 8 | 0.14 |
| (1,2153) | 1:168:A:SER:HB2 | 1:169:A:ASN:HA | 15 | 0.14 |
| (1,2153) | 1:168:A:SER:HB3 | 1:169:A:ASN:HA | 15 | 0.14 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD11 | 16 | 0.14 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD12 | 16 | 0.14 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD13 | 16 | 0.14 |
| (1,2118) | 1:10:A:ILE:HG13 | 1:159:A:GLN:H | 6 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2118) | 1:10:A:ILE:HG13 | 1:159:A:GLN:H | 12 | 0.14 |
| (1,2115) | 1:10:A:ILE:H | 1:10:A:ILE:HG13 | 11 | 0.14 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB2 | 15 | 0.14 |
| (1,2092) | 1:161:A:ASN:HD21 | 1:163:A:GLN:HB3 | 15 | 0.14 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG11 | 5 | 0.14 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG12 | 5 | 0.14 |
| (1,2042) | 1:27:A:SER:HB2 | 1:61:A:VAL:HG13 | 5 | 0.14 |
| (1,2009) | 1:48:A:GLN:HB3 | 1:49:A:LYS:H | 8 | 0.14 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 17 | 0.14 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 10 | 0.14 |
| (1,1930) | 1:186:A:GLU:HB3 | 1:187:A:LYS:H | 4 | 0.14 |
| (1,1920) | 1:31:A:PRO:HA | 1:96:A:GLN:HE21 | 6 | 0.14 |
| (1,1898) | 1:96:A:GLN:HB3 | 1:97:A:LYS:HG2 | 7 | 0.14 |
| (1,1860) | 1:101:A:VAL:HB | 1:106:A:ASP:HB3 | 9 | 0.14 |
| (1,1860) | 1:101:A:VAL:HB | 1:106:A:ASP:HB3 | 14 | 0.14 |
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 2 | 0.14 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 3 | 0.14 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 10 | 0.14 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 20 | 0.14 |
| (1,1778) | 1:72:A:THR:HB | 1:73:A:GLN:HB3 | 10 | 0.14 |
| (1,1758) | 1:14:A:LYS:H | 1:14:A:LYS:HB3 | 8 | 0.14 |
| (1,1747) | 1:50:A:LEU:HB2 | 1:54:A:THR:HB | 4 | 0.14 |
| (1,1730) | 1:55:A:LYS:H | 1:55:A:LYS:HB3 | 13 | 0.14 |
| (1,1698) | 1:136:A:GLN:HB2 | 1:136:A:GLN:HG2 | 6 | 0.14 |
| (1,1693) | 1:136:A:GLN:H | 1:136:A:GLN:HG2 | 5 | 0.14 |
| (1,1693) | 1:136:A:GLN:H | 1:136:A:GLN:HG2 | 12 | 0.14 |
| (1,1693) | 1:136:A:GLN:H | 1:136:A:GLN:HG2 | 16 | 0.14 |
| (1,1693) | 1:136:A:GLN:H | 1:136:A:GLN:HG2 | 20 | 0.14 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG2 | 10 | 0.14 |
| (1,1692) | 1:48:A:GLN:HG2 | 1:49:A:LYS:HG3 | 10 | 0.14 |
| (1,1685) | 1:99:A:GLN:HA | 1:99:A:GLN:HG3 | 4 | 0.14 |
| (1,1643) | 1:154:A:VAL:HB | 1:158:A:TYR:HD1 | 14 | 0.14 |
| (1,1643) | 1:154:A:VAL:HB | 1:158:A:TYR:HD2 | 14 | 0.14 |
| (1,1632) | 1:31:A:PRO:HA | 1:96:A:GLN:HG2 | 12 | 0.14 |
| (1,1632) | 1:31:A:PRO:HA | 1:96:A:GLN:HG2 | 15 | 0.14 |
| (1,1624) | 1:33:A:CYS:HA | 1:150:A:PRO:HB2 | 18 | 0.14 |
| (1,1606) | 1:52:A:GLU:HG2 | 1:53:A:GLY:HA3 | 12 | 0.14 |
| (1,1606) | 1:52:A:GLU:HG3 | 1:53:A:GLY:HA3 | 12 | 0.14 |
| (1,1535) | 1:33:A:CYS:H | 1:34:A:TYR:HB2 | 19 | 0.14 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 13 | 0.14 |
| (1,1438) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HB2 | 16 | 0.14 |
| (1,1438) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HB2 | 16 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1438) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HB2 | 16 | 0.14 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 10 | 0.14 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 10 | 0.14 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 10 | 0.14 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 16 | 0.14 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 16 | 0.14 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 16 | 0.14 |
| (1,1333) | 1:67:A:LEU:HD11 | 1:70:A:ASP:HB3 | 6 | 0.14 |
| (1,1333) | 1:67:A:LEU:HD12 | 1:70:A:ASP:HB3 | 6 | 0.14 |
| (1,1333) | 1:67:A:LEU:HD13 | 1:70:A:ASP:HB3 | 6 | 0.14 |
| (1,1328) | 1:106:A:ASP:HB3 | 1:107:A:ILE:HG13 | 10 | 0.14 |
| (1,1258) | 1:163:A:GLN:HG2 | 1:164:A:GLY:HA3 | 7 | 0.14 |
| (1,1258) | 1:163:A:GLN:HG3 | 1:164:A:GLY:HA3 | 7 | 0.14 |
| (1,1213) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE21 | 19 | 0.14 |
| (1,1213) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE21 | 19 | 0.14 |
| (1,1213) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE21 | 19 | 0.14 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 11 | 0.14 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 15 | 0.14 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 16 | 0.14 |
| (1,1116) | 1:61:A:VAL:HG11 | 1:63:A:PHE:H | 7 | 0.14 |
| (1,1116) | 1:61:A:VAL:HG12 | 1:63:A:PHE:H | 7 | 0.14 |
| (1,1116) | 1:61:A:VAL:HG13 | 1:63:A:PHE:H | 7 | 0.14 |
| (1,1102) | 1:9:A:TYR:H | 1:184:A:LEU:HD21 | 16 | 0.14 |
| (1,1102) | 1:9:A:TYR:H | 1:184:A:LEU:HD22 | 16 | 0.14 |
| (1,1102) | 1:9:A:TYR:H | 1:184:A:LEU:HD23 | 16 | 0.14 |
| (1,1080) | 1:34:A:TYR:HD1 | 1:38:A:GLU:H | 6 | 0.14 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 12 | 0.14 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 1 | 0.14 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 1 | 0.14 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 7 | 0.14 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 7 | 0.14 |
| (1,938) | 1:112:A:VAL:HG11 | 1:118:A:GLY:H | 6 | 0.14 |
| (1,938) | 1:112:A:VAL:HG12 | 1:118:A:GLY:H | 6 | 0.14 |
| (1,938) | 1:112:A:VAL:HG13 | 1:118:A:GLY:H | 6 | 0.14 |
| (1,883) | 1:49:A:LYS:H | 1:49:A:LYS:HD3 | 6 | 0.14 |
| (1,606) | 1:137:A:GLN:H | 1:137:A:GLN:HG2 | 8 | 0.14 |
| (1,606) | 1:137:A:GLN:H | 1:137:A:GLN:HG2 | 16 | 0.14 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 3 | 0.14 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 3 | 0.14 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 3 | 0.14 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 9 | 0.14 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 9 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 9 | 0.14 |
| (1,568) | 1:49:A:LYS:HA | 1:50:A:LEU:H | 3 | 0.14 |
| (1,555) | 1:174:A:VAL:HG21 | 1:178:A:ALA:H | 4 | 0.14 |
| (1,555) | 1:174:A:VAL:HG22 | 1:178:A:ALA:H | 4 | 0.14 |
| (1,555) | 1:174:A:VAL:HG23 | 1:178:A:ALA:H | 4 | 0.14 |
| (1,555) | 1:174:A:VAL:HG21 | 1:178:A:ALA:H | 11 | 0.14 |
| (1,555) | 1:174:A:VAL:HG22 | 1:178:A:ALA:H | 11 | 0.14 |
| (1,555) | 1:174:A:VAL:HG23 | 1:178:A:ALA:H | 11 | 0.14 |
| (1,555) | 1:174:A:VAL:HG21 | 1:178:A:ALA:H | 19 | 0.14 |
| (1,555) | 1:174:A:VAL:HG22 | 1:178:A:ALA:H | 19 | 0.14 |
| (1,555) | 1:174:A:VAL:HG23 | 1:178:A:ALA:H | 19 | 0.14 |
| (1,553) | 1:42:A:VAL:HG21 | 1:46:A:VAL:H | 3 | 0.14 |
| (1,553) | 1:42:A:VAL:HG22 | 1:46:A:VAL:H | 3 | 0.14 |
| (1,553) | 1:42:A:VAL:HG23 | 1:46:A:VAL:H | 3 | 0.14 |
| (1,479) | 1:122:A:ASP:HB3 | 1:124:A:ALA:H | 16 | 0.14 |
| (1,476) | 1:2:A:GLN:HB2 | 1:3:A:ILE:H | 3 | 0.14 |
| (1,476) | 1:2:A:GLN:HB2 | 1:3:A:ILE:H | 4 | 0.14 |
| (1,441) | 1:34:A:TYR:HE1 | 1:92:A:PHE:H | 20 | 0.14 |
| (1,380) | 1:138:A:GLU:H | 1:138:A:GLU:HG3 | 16 | 0.14 |
| (1,353) | 1:108:A:ARG:HG3 | 1:112:A:VAL:H | 19 | 0.14 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 12 | 0.14 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 12 | 0.14 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 12 | 0.14 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 7 | 0.14 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 7 | 0.14 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 7 | 0.14 |
| (1,300) | 1:130:A:VAL:HG21 | 1:131:A:LYS:H | 3 | 0.14 |
| (1,300) | 1:130:A:VAL:HG22 | 1:131:A:LYS:H | 3 | 0.14 |
| (1,300) | 1:130:A:VAL:HG23 | 1:131:A:LYS:H | 3 | 0.14 |
| (1,138) | 1:80:A:ALA:H | 1:81:A:LEU:HA | 5 | 0.14 |
| (1,138) | 1:80:A:ALA:H | 1:81:A:LEU:HA | 13 | 0.14 |
| (1,138) | 1:80:A:ALA:H | 1:81:A:LEU:HA | 15 | 0.14 |
| (1,102) | 1:50:A:LEU:HD21 | 1:56:A:MET:H | 16 | 0.14 |
| (1,102) | 1:50:A:LEU:HD22 | 1:56:A:MET:H | 16 | 0.14 |
| (1,102) | 1:50:A:LEU:HD23 | 1:56:A:MET:H | 16 | 0.14 |
| (1,67) | 1:26:A:PHE:H | 1:59:A:TYR:H | 6 | 0.14 |
| (1,62) | 1:102:A:GLN:H | 1:102:A:GLN:HG2 | 6 | 0.14 |
| (1,3531) | 1:58:A:LYS:H | 1:75:A:TRP:HZ2 | 3 | 0.13 |
| (1,3530) | 1:73:A:GLN:HE22 | 1:125:A:TRP:HZ2 | 17 | 0.13 |
| (1,3529) | 1:58:A:LYS:HB2 | 1:75:A:TRP:HZ2 | 2 | 0.13 |
| (1,3529) | 1:58:A:LYS:HB3 | 1:75:A:TRP:HZ2 | 2 | 0.13 |
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 6 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE1 | 2 | 0.13 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE2 | 2 | 0.13 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE1 | 10 | 0.13 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE2 | 10 | 0.13 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE1 | 16 | 0.13 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE2 | 16 | 0.13 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 4 | 0.13 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 4 | 0.13 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 5 | 0.13 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 5 | 0.13 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 8 | 0.13 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 8 | 0.13 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 10 | 0.13 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 10 | 0.13 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 11 | 0.13 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 11 | 0.13 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 12 | 0.13 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 12 | 0.13 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 13 | 0.13 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 13 | 0.13 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE1 | 17 | 0.13 |
| (1,3509) | 1:158:A:TYR:HA | 1:158:A:TYR:HE2 | 17 | 0.13 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE1 | 8 | 0.13 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE2 | 8 | 0.13 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE1 | 8 | 0.13 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE2 | 8 | 0.13 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE1 | 12 | 0.13 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE2 | 12 | 0.13 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE1 | 12 | 0.13 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE2 | 12 | 0.13 |
| (1,3495) | 1:23:A:LEU:HD21 | 1:59:A:TYR:HE1 | 12 | 0.13 |
| (1,3495) | 1:23:A:LEU:HD21 | 1:59:A:TYR:HE2 | 12 | 0.13 |
| (1,3495) | 1:23:A:LEU:HD22 | 1:59:A:TYR:HE1 | 12 | 0.13 |
| (1,3495) | 1:23:A:LEU:HD22 | 1:59:A:TYR:HE2 | 12 | 0.13 |
| (1,3495) | 1:23:A:LEU:HD23 | 1:59:A:TYR:HE1 | 12 | 0.13 |
| (1,3495) | 1:23:A:LEU:HD23 | 1:59:A:TYR:HE2 | 12 | 0.13 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB2 | 7 | 0.13 |
| (1,3493) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HB3 | 7 | 0.13 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB2 | 7 | 0.13 |
| (1,3493) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HB3 | 7 | 0.13 |
| (1,3487) | 1:29:A:TYR:HE1 | 1:67:A:LEU:H | 19 | 0.13 |
| (1,3487) | 1:29:A:TYR:HE2 | 1:67:A:LEU:H | 19 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE1 | 1 | 0.13 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE2 | 1 | 0.13 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE1 | 10 | 0.13 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE2 | 10 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE1 | 3 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE2 | 3 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE1 | 3 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE2 | 3 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE1 | 3 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE2 | 3 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE1 | 5 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE2 | 5 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE1 | 5 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE2 | 5 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE1 | 5 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE2 | 5 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE1 | 20 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE2 | 20 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE1 | 20 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE2 | 20 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE1 | 20 | 0.13 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE2 | 20 | 0.13 |
| (1,3481) | 1:29:A:TYR:HE1 | 1:67:A:LEU:HA | 12 | 0.13 |
| (1,3481) | 1:29:A:TYR:HE2 | 1:67:A:LEU:HA | 12 | 0.13 |
| (1,3480) | 1:32:A:HIS:HD2 | 1:150:A:PRO:HG3 | 1 | 0.13 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE1 | 8 | 0.13 |
| (1,3475) | 1:152:A:MET:HA | 1:153:A:TYR:HE2 | 8 | 0.13 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE1 | 10 | 0.13 |
| (1,3473) | 1:153:A:TYR:H | 1:153:A:TYR:HE2 | 10 | 0.13 |
| (1,3463) | 1:77:A:VAL:H | 1:125:A:TRP:HE3 | 1 | 0.13 |
| (1,3463) | 1:77:A:VAL:H | 1:125:A:TRP:HE3 | 2 | 0.13 |
| (1,3463) | 1:77:A:VAL:H | 1:125:A:TRP:HE3 | 4 | 0.13 |
| (1,3463) | 1:77:A:VAL:H | 1:125:A:TRP:HE3 | 14 | 0.13 |
| (1,3463) | 1:77:A:VAL:H | 1:125:A:TRP:HE3 | 15 | 0.13 |
| (1,3461) | 1:75:A:TRP:HB3 | 1:75:A:TRP:HE3 | 2 | 0.13 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 4 | 0.13 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 10 | 0.13 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 11 | 0.13 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 16 | 0.13 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 18 | 0.13 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 1 | 0.13 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 3 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 5 | 0.13 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 8 | 0.13 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 14 | 0.13 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 18 | 0.13 |
| (1,3450) | 1:75:A:TRP:HA | 1:75:A:TRP:HZ3 | 19 | 0.13 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 9 | 0.13 |
| (1,3448) | 1:77:A:VAL:HB | 1:125:A:TRP:HZ3 | 20 | 0.13 |
| (1,3436) | 1:75:A:TRP:HH2 | 1:87:A:ILE:HD11 | 18 | 0.13 |
| (1,3436) | 1:75:A:TRP:HH2 | 1:87:A:ILE:HD12 | 18 | 0.13 |
| (1,3436) | 1:75:A:TRP:HH2 | 1:87:A:ILE:HD13 | 18 | 0.13 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG2 | 2 | 0.13 |
| (1,3433) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HG3 | 2 | 0.13 |
| (1,3422) | 1:60:A:HIS:H | 1:75:A:TRP:HD1 | 16 | 0.13 |
| (1,3422) | 1:60:A:HIS:H | 1:75:A:TRP:HD1 | 18 | 0.13 |
| (1,3422) | 1:60:A:HIS:H | 1:75:A:TRP:HD1 | 20 | 0.13 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD11 | 17 | 0.13 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD12 | 17 | 0.13 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD13 | 17 | 0.13 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD11 | 17 | 0.13 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD12 | 17 | 0.13 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD13 | 17 | 0.13 |
| (1,3407) | 1:59:A:TYR:HD1 | 1:60:A:HIS:H | 8 | 0.13 |
| (1,3407) | 1:59:A:TYR:HD2 | 1:60:A:HIS:H | 8 | 0.13 |
| (1,3407) | 1:59:A:TYR:HD1 | 1:60:A:HIS:H | 9 | 0.13 |
| (1,3407) | 1:59:A:TYR:HD2 | 1:60:A:HIS:H | 9 | 0.13 |
| (1,3407) | 1:59:A:TYR:HD1 | 1:60:A:HIS:H | 10 | 0.13 |
| (1,3407) | 1:59:A:TYR:HD2 | 1:60:A:HIS:H | 10 | 0.13 |
| (1,3402) | 1:26:A:PHE:H | 1:26:A:PHE:HD1 | 3 | 0.13 |
| (1,3402) | 1:26:A:PHE:H | 1:26:A:PHE:HD2 | 3 | 0.13 |
| (1,3392) | 1:128:A:PHE:HA | 1:128:A:PHE:HD2 | 9 | 0.13 |
| (1,3392) | 1:128:A:PHE:HA | 1:128:A:PHE:HD2 | 11 | 0.13 |
| (1,3388) | 1:34:A:TYR:HD1 | 1:92:A:PHE:HA | 3 | 0.13 |
| (1,3388) | 1:34:A:TYR:HD2 | 1:92:A:PHE:HA | 3 | 0.13 |
| (1,3388) | 1:34:A:TYR:HD1 | 1:92:A:PHE:HA | 8 | 0.13 |
| (1,3388) | 1:34:A:TYR:HD2 | 1:92:A:PHE:HA | 8 | 0.13 |
| (1,3382) | 1:34:A:TYR:HD1 | 1:35:A:GLN:HG2 | 18 | 0.13 |
| (1,3382) | 1:34:A:TYR:HD1 | 1:35:A:GLN:HG3 | 18 | 0.13 |
| (1,3382) | 1:34:A:TYR:HD2 | 1:35:A:GLN:HG2 | 18 | 0.13 |
| (1,3382) | 1:34:A:TYR:HD2 | 1:35:A:GLN:HG3 | 18 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD1 | 12 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD2 | 12 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD1 | 12 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD2 | 12 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD1 | 12 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD2 | 12 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD1 | 15 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD2 | 15 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD1 | 15 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD2 | 15 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD1 | 15 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD2 | 15 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD1 | 17 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD2 | 17 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD1 | 17 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD2 | 17 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD1 | 17 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD2 | 17 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD1 | 18 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD2 | 18 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD1 | 18 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD2 | 18 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD1 | 18 | 0.13 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD2 | 18 | 0.13 |
| (1,3371) | 1:167:A:THR:HG21 | 1:173:A:PHE:HD1 | 6 | 0.13 |
| (1,3371) | 1:167:A:THR:HG21 | 1:173:A:PHE:HD2 | 6 | 0.13 |
| (1,3371) | 1:167:A:THR:HG22 | 1:173:A:PHE:HD1 | 6 | 0.13 |
| (1,3371) | 1:167:A:THR:HG22 | 1:173:A:PHE:HD2 | 6 | 0.13 |
| (1,3371) | 1:167:A:THR:HG23 | 1:173:A:PHE:HD1 | 6 | 0.13 |
| (1,3371) | 1:167:A:THR:HG23 | 1:173:A:PHE:HD2 | 6 | 0.13 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD1 | 6 | 0.13 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD2 | 6 | 0.13 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD1 | 11 | 0.13 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD2 | 11 | 0.13 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD1 | 19 | 0.13 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD2 | 19 | 0.13 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD1 | 20 | 0.13 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD2 | 20 | 0.13 |
| (1,3336) | 1:92:A:PHE:HD1 | 1:96:A:GLN:HG2 | 2 | 0.13 |
| (1,3336) | 1:92:A:PHE:HD2 | 1:96:A:GLN:HG2 | 2 | 0.13 |
| (1,3336) | 1:92:A:PHE:HD1 | 1:96:A:GLN:HG2 | 5 | 0.13 |
| (1,3336) | 1:92:A:PHE:HD2 | 1:96:A:GLN:HG2 | 5 | 0.13 |
| (1,3336) | 1:92:A:PHE:HD1 | 1:96:A:GLN:HG2 | 10 | 0.13 |
| (1,3336) | 1:92:A:PHE:HD2 | 1:96:A:GLN:HG2 | 10 | 0.13 |
| (1,3325) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HD1 | 12 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3325) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HD2 | 12 | 0.13 |
| (1,3325) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HD1 | 12 | 0.13 |
| (1,3325) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HD2 | 12 | 0.13 |
| (1,3325) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HD1 | 12 | 0.13 |
| (1,3325) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HD2 | 12 | 0.13 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD1 | 9 | 0.13 |
| (1,3322) | 1:4:A:THR:HA | 1:9:A:TYR:HD2 | 9 | 0.13 |
| (1,3305) | 1:38:A:GLU:H | 1:41:A:HIS:HE1 | 15 | 0.13 |
| (1,3305) | 1:38:A:GLU:H | 1:41:A:HIS:HE1 | 20 | 0.13 |
| (1,3286) | 1:81:A:LEU:HB2 | 1:82:A:GLY:HA3 | 10 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 2 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 2 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 2 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 2 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 2 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 2 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 5 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 5 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 5 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 5 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 5 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 5 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 6 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 6 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 6 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 6 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 6 | 0.13 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 6 | 0.13 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE1 | 5 | 0.13 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE2 | 5 | 0.13 |
| (1,3071) | 1:47:A:ARG:H | 1:56:A:MET:HE3 | 5 | 0.13 |
| (1,3061) | 1:49:A:LYS:HB3 | 1:178:A:ALA:HB1 | 19 | 0.13 |
| (1,3061) | 1:49:A:LYS:HB3 | 1:178:A:ALA:HB2 | 19 | 0.13 |
| (1,3061) | 1:49:A:LYS:HB3 | 1:178:A:ALA:HB3 | 19 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG21 | 1:175:A:ALA:HB1 | 4 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG21 | 1:175:A:ALA:HB2 | 4 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG21 | 1:175:A:ALA:HB3 | 4 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG22 | 1:175:A:ALA:HB1 | 4 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG22 | 1:175:A:ALA:HB2 | 4 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG22 | 1:175:A:ALA:HB3 | 4 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG23 | 1:175:A:ALA:HB1 | 4 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG23 | 1:175:A:ALA:HB2 | 4 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3053) | 1:172:A:VAL:HG23 | 1:175:A:ALA:HB3 | 4 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG21 | 1:175:A:ALA:HB1 | 19 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG21 | 1:175:A:ALA:HB2 | 19 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG21 | 1:175:A:ALA:HB3 | 19 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG22 | 1:175:A:ALA:HB1 | 19 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG22 | 1:175:A:ALA:HB2 | 19 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG22 | 1:175:A:ALA:HB3 | 19 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG23 | 1:175:A:ALA:HB1 | 19 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG23 | 1:175:A:ALA:HB2 | 19 | 0.13 |
| (1,3053) | 1:172:A:VAL:HG23 | 1:175:A:ALA:HB3 | 19 | 0.13 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG21 | 16 | 0.13 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG22 | 16 | 0.13 |
| (1,3030) | 1:80:A:ALA:HB1 | 1:130:A:VAL:HG23 | 16 | 0.13 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG21 | 16 | 0.13 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG22 | 16 | 0.13 |
| (1,3030) | 1:80:A:ALA:HB2 | 1:130:A:VAL:HG23 | 16 | 0.13 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG21 | 16 | 0.13 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG22 | 16 | 0.13 |
| (1,3030) | 1:80:A:ALA:HB3 | 1:130:A:VAL:HG23 | 16 | 0.13 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB1 | 2 | 0.13 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB2 | 2 | 0.13 |
| (1,3022) | 1:122:A:ASP:HB3 | 1:123:A:ALA:HB3 | 2 | 0.13 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD21 | 17 | 0.13 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD22 | 17 | 0.13 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD23 | 17 | 0.13 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD21 | 4 | 0.13 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD22 | 4 | 0.13 |
| (1,2999) | 1:140:A:ALA:HB1 | 1:146:A:LEU:HD23 | 4 | 0.13 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD21 | 4 | 0.13 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD22 | 4 | 0.13 |
| (1,2999) | 1:140:A:ALA:HB2 | 1:146:A:LEU:HD23 | 4 | 0.13 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD21 | 4 | 0.13 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD22 | 4 | 0.13 |
| (1,2999) | 1:140:A:ALA:HB3 | 1:146:A:LEU:HD23 | 4 | 0.13 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB1 | 20 | 0.13 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB2 | 20 | 0.13 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB3 | 20 | 0.13 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB1 | 20 | 0.13 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB2 | 20 | 0.13 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB3 | 20 | 0.13 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD11 | 15 | 0.13 |
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD12 | 15 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2972) | 1:141:A:ALA:HA | 1:146:A:LEU:HD13 | 15 | 0.13 |
| (1,2890) | 1:71:A:LEU:HD21 | 1:74:A:ALA:HB1 | 6 | 0.13 |
| (1,2890) | 1:71:A:LEU:HD21 | 1:74:A:ALA:HB2 | 6 | 0.13 |
| (1,2890) | 1:71:A:LEU:HD21 | 1:74:A:ALA:HB3 | 6 | 0.13 |
| (1,2890) | 1:71:A:LEU:HD22 | 1:74:A:ALA:HB1 | 6 | 0.13 |
| (1,2890) | 1:71:A:LEU:HD22 | 1:74:A:ALA:HB2 | 6 | 0.13 |
| (1,2890) | 1:71:A:LEU:HD22 | 1:74:A:ALA:HB3 | 6 | 0.13 |
| (1,2890) | 1:71:A:LEU:HD23 | 1:74:A:ALA:HB1 | 6 | 0.13 |
| (1,2890) | 1:71:A:LEU:HD23 | 1:74:A:ALA:HB2 | 6 | 0.13 |
| (1,2890) | 1:71:A:LEU:HD23 | 1:74:A:ALA:HB3 | 6 | 0.13 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE1 | 14 | 0.13 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE2 | 14 | 0.13 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE3 | 14 | 0.13 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 11 | 0.13 |
| (1,2847) | 1:2:A:GLN:HA | 1:2:A:GLN:HB3 | 5 | 0.13 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG11 | 8 | 0.13 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG12 | 8 | 0.13 |
| (1,2841) | 1:41:A:HIS:HA | 1:42:A:VAL:HG13 | 8 | 0.13 |
| (1,2838) | 1:34:A:TYR:HE1 | 1:38:A:GLU:HA | 6 | 0.13 |
| (1,2838) | 1:34:A:TYR:HE2 | 1:38:A:GLU:HA | 6 | 0.13 |
| (1,2838) | 1:34:A:TYR:HE1 | 1:38:A:GLU:HA | 12 | 0.13 |
| (1,2838) | 1:34:A:TYR:HE2 | 1:38:A:GLU:HA | 12 | 0.13 |
| (1,2838) | 1:34:A:TYR:HE1 | 1:38:A:GLU:HA | 19 | 0.13 |
| (1,2838) | 1:34:A:TYR:HE2 | 1:38:A:GLU:HA | 19 | 0.13 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG11 | 16 | 0.13 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG12 | 16 | 0.13 |
| (1,2793) | 1:87:A:ILE:HG21 | 1:116:A:VAL:HG13 | 16 | 0.13 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG11 | 16 | 0.13 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG12 | 16 | 0.13 |
| (1,2793) | 1:87:A:ILE:HG22 | 1:116:A:VAL:HG13 | 16 | 0.13 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG11 | 16 | 0.13 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG12 | 16 | 0.13 |
| (1,2793) | 1:87:A:ILE:HG23 | 1:116:A:VAL:HG13 | 16 | 0.13 |
| (1,2787) | 1:86:A:LYS:H | 1:87:A:ILE:HG21 | 7 | 0.13 |
| (1,2787) | 1:86:A:LYS:H | 1:87:A:ILE:HG22 | 7 | 0.13 |
| (1,2787) | 1:86:A:LYS:H | 1:87:A:ILE:HG23 | 7 | 0.13 |
| (1,2766) | 1:39:A:VAL:HG21 | 1:40:A:LEU:H | 18 | 0.13 |
| (1,2766) | 1:39:A:VAL:HG22 | 1:40:A:LEU:H | 18 | 0.13 |
| (1,2766) | 1:39:A:VAL:HG23 | 1:40:A:LEU:H | 18 | 0.13 |
| (1,2753) | 1:61:A:VAL:HG11 | 1:62:A:GLU:HA | 20 | 0.13 |
| (1,2753) | 1:61:A:VAL:HG12 | 1:62:A:GLU:HA | 20 | 0.13 |
| (1,2753) | 1:61:A:VAL:HG13 | 1:62:A:GLU:HA | 20 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG11 | 15 | 0.13 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG12 | 15 | 0.13 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG13 | 15 | 0.13 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG21 | 16 | 0.13 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG22 | 16 | 0.13 |
| (1,2675) | 1:160:A:LEU:HD21 | 1:180:A:THR:HG23 | 16 | 0.13 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG21 | 16 | 0.13 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG22 | 16 | 0.13 |
| (1,2675) | 1:160:A:LEU:HD22 | 1:180:A:THR:HG23 | 16 | 0.13 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG21 | 16 | 0.13 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG22 | 16 | 0.13 |
| (1,2675) | 1:160:A:LEU:HD23 | 1:180:A:THR:HG23 | 16 | 0.13 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG21 | 3 | 0.13 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG22 | 3 | 0.13 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG23 | 3 | 0.13 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG21 | 9 | 0.13 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG22 | 9 | 0.13 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG23 | 9 | 0.13 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG21 | 17 | 0.13 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG22 | 17 | 0.13 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG23 | 17 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG21 | 8 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG22 | 8 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG23 | 8 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG21 | 8 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG22 | 8 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG23 | 8 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG21 | 8 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG22 | 8 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG23 | 8 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG21 | 11 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG22 | 11 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG23 | 11 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG21 | 11 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG22 | 11 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG23 | 11 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG21 | 11 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG22 | 11 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG23 | 11 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG21 | 17 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG22 | 17 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG23 | 17 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG21 | 17 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG22 | 17 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG23 | 17 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG21 | 17 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG22 | 17 | 0.13 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG23 | 17 | 0.13 |
| (1,2632) | 1:101:A:VAL:HG21 | 1:107:A:ILE:H | 6 | 0.13 |
| (1,2632) | 1:101:A:VAL:HG22 | 1:107:A:ILE:H | 6 | 0.13 |
| (1,2632) | 1:101:A:VAL:HG23 | 1:107:A:ILE:H | 6 | 0.13 |
| (1,2632) | 1:101:A:VAL:HG21 | 1:107:A:ILE:H | 18 | 0.13 |
| (1,2632) | 1:101:A:VAL:HG22 | 1:107:A:ILE:H | 18 | 0.13 |
| (1,2632) | 1:101:A:VAL:HG23 | 1:107:A:ILE:H | 18 | 0.13 |
| (1,2630) | 1:101:A:VAL:HG21 | 1:102:A:GLN:H | 5 | 0.13 |
| (1,2630) | 1:101:A:VAL:HG22 | 1:102:A:GLN:H | 5 | 0.13 |
| (1,2630) | 1:101:A:VAL:HG23 | 1:102:A:GLN:H | 5 | 0.13 |
| (1,2630) | 1:101:A:VAL:HG21 | 1:102:A:GLN:H | 7 | 0.13 |
| (1,2630) | 1:101:A:VAL:HG22 | 1:102:A:GLN:H | 7 | 0.13 |
| (1,2630) | 1:101:A:VAL:HG23 | 1:102:A:GLN:H | 7 | 0.13 |
| (1,2622) | 1:149:A:VAL:HA | 1:151:A:ALA:H | 16 | 0.13 |
| (1,2622) | 1:149:A:VAL:HA | 1:151:A:ALA:H | 20 | 0.13 |
| (1,2621) | 1:101:A:VAL:HG21 | 1:106:A:ASP:H | 1 | 0.13 |
| (1,2621) | 1:101:A:VAL:HG22 | 1:106:A:ASP:H | 1 | 0.13 |
| (1,2621) | 1:101:A:VAL:HG23 | 1:106:A:ASP:H | 1 | 0.13 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG21 | 7 | 0.13 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG22 | 7 | 0.13 |
| (1,2613) | 1:10:A:ILE:HA | 1:11:A:THR:HG23 | 7 | 0.13 |
| (1,2596) | 1:63:A:PHE:HA | 1:64:A:LEU:H | 12 | 0.13 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG21 | 2 | 0.13 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG22 | 2 | 0.13 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG23 | 2 | 0.13 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG21 | 2 | 0.13 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG22 | 2 | 0.13 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG23 | 2 | 0.13 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG21 | 2 | 0.13 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG22 | 2 | 0.13 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG23 | 2 | 0.13 |
| (1,2519) | 1:127:A:SER:HA | 1:128:A:PHE:HB2 | 3 | 0.13 |
| (1,2519) | 1:127:A:SER:HA | 1:128:A:PHE:HB2 | 5 | 0.13 |
| (1,2519) | 1:127:A:SER:HA | 1:128:A:PHE:HB2 | 9 | 0.13 |
| (1,2519) | 1:127:A:SER:HA | 1:128:A:PHE:HB2 | 11 | 0.13 |
| (1,2484) | 1:183:A:GLN:HA | 1:183:A:GLN:HB2 | 2 | 0.13 |
| (1,2484) | 1:183:A:GLN:HA | 1:183:A:GLN:HB2 | 4 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2422) | 1:47:A:ARG:HA | 1:50:A:LEU:HG | 7 | 0.13 |
| (1,2315) | 1:46:A:VAL:HG21 | 1:50:A:LEU:HG | 6 | 0.13 |
| (1,2315) | 1:46:A:VAL:HG22 | 1:50:A:LEU:HG | 6 | 0.13 |
| (1,2315) | 1:46:A:VAL:HG23 | 1:50:A:LEU:HG | 6 | 0.13 |
| (1,2291) | 1:117:A:LYS:HG3 | 1:120:A:ASP:H | 10 | 0.13 |
| (1,2274) | 1:4:A:THR:HA | 1:7:A:LYS:HB2 | 7 | 0.13 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 8 | 0.13 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 8 | 0.13 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 8 | 0.13 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 8 | 0.13 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 8 | 0.13 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 8 | 0.13 |
| (1,2240) | 1:172:A:VAL:H | 1:173:A:PHE:HA | 1 | 0.13 |
| (1,2214) | 1:120:A:ASP:HB2 | 1:121:A:TYR:HA | 7 | 0.13 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE1 | 5 | 0.13 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE2 | 5 | 0.13 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE3 | 5 | 0.13 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE1 | 5 | 0.13 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE2 | 5 | 0.13 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE3 | 5 | 0.13 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE1 | 10 | 0.13 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE2 | 10 | 0.13 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE3 | 10 | 0.13 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE1 | 10 | 0.13 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE2 | 10 | 0.13 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE3 | 10 | 0.13 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE1 | 13 | 0.13 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE2 | 13 | 0.13 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE3 | 13 | 0.13 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE1 | 13 | 0.13 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE2 | 13 | 0.13 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE3 | 13 | 0.13 |
| (1,2168) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HG2 | 3 | 0.13 |
| (1,2168) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HG2 | 3 | 0.13 |
| (1,2167) | 1:4:A:THR:H | 1:8:A:GLN:HB3 | 10 | 0.13 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD11 | 2 | 0.13 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD12 | 2 | 0.13 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD13 | 2 | 0.13 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 4 | 0.13 |
| (1,1981) | 1:187:A:LYS:H | 1:187:A:LYS:HD3 | 4 | 0.13 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 7 | 0.13 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 15 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1867) | 1:37:A:GLU:HB2 | 1:38:A:GLU:HA | 15 | 0.13 |
| (1,1843) | 1:60:A:HIS:HB2 | 1:72:A:THR:HA | 14 | 0.13 |
| (1,1832) | 1:124:A:ALA:HB1 | 1:130:A:VAL:HB | 2 | 0.13 |
| (1,1832) | 1:124:A:ALA:HB2 | 1:130:A:VAL:HB | 2 | 0.13 |
| (1,1832) | 1:124:A:ALA:HB3 | 1:130:A:VAL:HB | 2 | 0.13 |
| (1,1832) | 1:124:A:ALA:HB1 | 1:130:A:VAL:HB | 5 | 0.13 |
| (1,1832) | 1:124:A:ALA:HB2 | 1:130:A:VAL:HB | 5 | 0.13 |
| (1,1832) | 1:124:A:ALA:HB3 | 1:130:A:VAL:HB | 5 | 0.13 |
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 11 | 0.13 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD1 | 13 | 0.13 |
| (1,1802) | 1:162:A:PRO:HB2 | 1:177:A:TYR:HD2 | 13 | 0.13 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 4 | 0.13 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 12 | 0.13 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 13 | 0.13 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 14 | 0.13 |
| (1,1800) | 1:161:A:ASN:HA | 1:162:A:PRO:HB2 | 17 | 0.13 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 6 | 0.13 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 14 | 0.13 |
| (1,1785) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD2 | 4 | 0.13 |
| (1,1785) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD2 | 12 | 0.13 |
| (1,1758) | 1:14:A:LYS:H | 1:14:A:LYS:HB3 | 9 | 0.13 |
| (1,1693) | 1:136:A:GLN:H | 1:136:A:GLN:HG2 | 4 | 0.13 |
| (1,1676) | 1:163:A:GLN:H | 1:163:A:GLN:HG2 | 9 | 0.13 |
| (1,1676) | 1:163:A:GLN:H | 1:163:A:GLN:HG3 | 9 | 0.13 |
| (1,1663) | 1:72:A:THR:HG21 | 1:138:A:GLU:HG3 | 17 | 0.13 |
| (1,1663) | 1:72:A:THR:HG22 | 1:138:A:GLU:HG3 | 17 | 0.13 |
| (1,1663) | 1:72:A:THR:HG23 | 1:138:A:GLU:HG3 | 17 | 0.13 |
| (1,1641) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HB | 10 | 0.13 |
| (1,1641) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HB | 10 | 0.13 |
| (1,1641) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HB | 10 | 0.13 |
| (1,1632) | 1:31:A:PRO:HA | 1:96:A:GLN:HG2 | 8 | 0.13 |
| (1,1604) | 1:61:A:VAL:HA | 1:62:A:GLU:HG2 | 14 | 0.13 |
| (1,1565) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 3 | 0.13 |
| (1,1508) | 1:15:A:PRO:HA | 1:16:A:ILE:HB | 15 | 0.13 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG11 | 12 | 0.13 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG12 | 12 | 0.13 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG13 | 12 | 0.13 |
| (1,1474) | 1:161:A:ASN:HB2 | 1:161:A:ASN:HD22 | 10 | 0.13 |
| (1,1438) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HB2 | 11 | 0.13 |
| (1,1438) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HB2 | 11 | 0.13 |
| (1,1438) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HB2 | 11 | 0.13 |
| (1,1438) | 1:112:A:VAL:HG21 | 1:113:A:ASP:HB2 | 14 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1438) | 1:112:A:VAL:HG22 | 1:113:A:ASP:HB2 | 14 | 0.13 |
| (1,1438) | 1:112:A:VAL:HG23 | 1:113:A:ASP:HB2 | 14 | 0.13 |
| (1,1426) | 1:143:A:ASP:HB2 | 1:144:A:LEU:HG | 18 | 0.13 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB2 | 1 | 0.13 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB3 | 1 | 0.13 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB2 | 20 | 0.13 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB3 | 20 | 0.13 |
| (1,1331) | 1:70:A:ASP:HB3 | 1:72:A:THR:H | 7 | 0.13 |
| (1,1265) | 1:64:A:LEU:HB3 | 1:65:A:GLY:HA2 | 11 | 0.13 |
| (1,1213) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE21 | 13 | 0.13 |
| (1,1213) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE21 | 13 | 0.13 |
| (1,1213) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE21 | 13 | 0.13 |
| (1,1202) | 1:92:A:PHE:HD1 | 1:96:A:GLN:HE22 | 3 | 0.13 |
| (1,1202) | 1:92:A:PHE:HD2 | 1:96:A:GLN:HE22 | 3 | 0.13 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 14 | 0.13 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 5 | 0.13 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 5 | 0.13 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 13 | 0.13 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 19 | 0.13 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 20 | 0.13 |
| (1,985) | 1:93:A:GLU:HB2 | 1:95:A:VAL:H | 13 | 0.13 |
| (1,985) | 1:93:A:GLU:HB3 | 1:95:A:VAL:H | 13 | 0.13 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 4 | 0.13 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 4 | 0.13 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 10 | 0.13 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 10 | 0.13 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 13 | 0.13 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 13 | 0.13 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 15 | 0.13 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 15 | 0.13 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 17 | 0.13 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 17 | 0.13 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 18 | 0.13 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 18 | 0.13 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 7 | 0.13 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 7 | 0.13 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 7 | 0.13 |
| (1,815) | 1:91:A:MET:HB2 | 1:93:A:GLU:H | 10 | 0.13 |
| (1,747) | 1:118:A:GLY:HA2 | 1:119:A:GLU:H | 13 | 0.13 |
| (1,650) | 1:145:A:GLN:HA | 1:146:A:LEU:H | 3 | 0.13 |
| (1,570) | 1:50:A:LEU:H | 1:51:A:PRO:HD3 | 15 | 0.13 |
| (1,560) | 1:42:A:VAL:HG21 | 1:178:A:ALA:H | 17 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,560) | 1:42:A:VAL:HG22 | 1:178:A:ALA:H | 17 | 0.13 |
| (1,560) | 1:42:A:VAL:HG23 | 1:178:A:ALA:H | 17 | 0.13 |
| (1,529) | 1:127:A:SER:HB2 | 1:129:A:VAL:H | 8 | 0.13 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 2 | 0.13 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 2 | 0.13 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 2 | 0.13 |
| (1,311) | 1:77:A:VAL:HG21 | 1:78:A:ALA:H | 15 | 0.13 |
| (1,311) | 1:77:A:VAL:HG22 | 1:78:A:ALA:H | 15 | 0.13 |
| (1,311) | 1:77:A:VAL:HG23 | 1:78:A:ALA:H | 15 | 0.13 |
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 6 | 0.13 |
| (1,280) | 1:13:A:ASP:H | 1:14:A:LYS:HB2 | 11 | 0.13 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 8 | 0.13 |
| (1,221) | 1:169:A:ASN:HB3 | 1:170:A:MET:H | 3 | 0.13 |
| (1,165) | 1:67:A:LEU:H | 1:69:A:LYS:H | 13 | 0.13 |
| (1,138) | 1:80:A:ALA:H | 1:81:A:LEU:HA | 17 | 0.13 |
| (1,67) | 1:26:A:PHE:H | 1:59:A:TYR:H | 19 | 0.13 |
| (1,62) | 1:102:A:GLN:H | 1:102:A:GLN:HG2 | 1 | 0.13 |
| (1,62) | 1:102:A:GLN:H | 1:102:A:GLN:HG2 | 2 | 0.13 |
| (1,3525) | 1:70:A:ASP:HB2 | 1:125:A:TRP:HZ2 | 18 | 0.12 |
| (1,3521) | 1:162:A:PRO:HG2 | 1:177:A:TYR:HE1 | 1 | 0.12 |
| (1,3521) | 1:162:A:PRO:HG2 | 1:177:A:TYR:HE2 | 1 | 0.12 |
| (1,3521) | 1:162:A:PRO:HG3 | 1:177:A:TYR:HE1 | 1 | 0.12 |
| (1,3521) | 1:162:A:PRO:HG3 | 1:177:A:TYR:HE2 | 1 | 0.12 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE1 | 6 | 0.12 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE2 | 6 | 0.12 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE1 | 18 | 0.12 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE2 | 18 | 0.12 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE1 | 1 | 0.12 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE2 | 1 | 0.12 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE1 | 1 | 0.12 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE2 | 1 | 0.12 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE1 | 13 | 0.12 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE2 | 13 | 0.12 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE1 | 13 | 0.12 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE2 | 13 | 0.12 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE1 | 20 | 0.12 |
| (1,3505) | 1:157:A:LYS:HD2 | 1:158:A:TYR:HE2 | 20 | 0.12 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE1 | 20 | 0.12 |
| (1,3505) | 1:157:A:LYS:HD3 | 1:158:A:TYR:HE2 | 20 | 0.12 |
| (1,3489) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HA | 1 | 0.12 |
| (1,3489) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HA | 1 | 0.12 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG21 | 14 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG22 | 14 | 0.12 |
| (1,3488) | 1:29:A:TYR:HE1 | 1:95:A:VAL:HG23 | 14 | 0.12 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG21 | 14 | 0.12 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG22 | 14 | 0.12 |
| (1,3488) | 1:29:A:TYR:HE2 | 1:95:A:VAL:HG23 | 14 | 0.12 |
| (1,3487) | 1:29:A:TYR:HE1 | 1:67:A:LEU:H | 10 | 0.12 |
| (1,3487) | 1:29:A:TYR:HE2 | 1:67:A:LEU:H | 10 | 0.12 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE1 | 5 | 0.12 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE2 | 5 | 0.12 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE1 | 1 | 0.12 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE2 | 1 | 0.12 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE1 | 1 | 0.12 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE2 | 1 | 0.12 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE1 | 1 | 0.12 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE2 | 1 | 0.12 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE1 | 13 | 0.12 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE2 | 13 | 0.12 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE1 | 13 | 0.12 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE2 | 13 | 0.12 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE1 | 13 | 0.12 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE2 | 13 | 0.12 |
| (1,3481) | 1:29:A:TYR:HE1 | 1:67:A:LEU:HA | 18 | 0.12 |
| (1,3481) | 1:29:A:TYR:HE2 | 1:67:A:LEU:HA | 18 | 0.12 |
| (1,3476) | 1:153:A:TYR:HE1 | 1:159:A:GLN:HB3 | 1 | 0.12 |
| (1,3476) | 1:153:A:TYR:HE2 | 1:159:A:GLN:HB3 | 1 | 0.12 |
| (1,3463) | 1:77:A:VAL:H | 1:125:A:TRP:HE3 | 6 | 0.12 |
| (1,3463) | 1:77:A:VAL:H | 1:125:A:TRP:HE3 | 12 | 0.12 |
| (1,3461) | 1:75:A:TRP:HB3 | 1:75:A:TRP:HE3 | 4 | 0.12 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 6 | 0.12 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 9 | 0.12 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 12 | 0.12 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 17 | 0.12 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 20 | 0.12 |
| (1,3436) | 1:75:A:TRP:HH2 | 1:87:A:ILE:HD11 | 20 | 0.12 |
| (1,3436) | 1:75:A:TRP:HH2 | 1:87:A:ILE:HD12 | 20 | 0.12 |
| (1,3436) | 1:75:A:TRP:HH2 | 1:87:A:ILE:HD13 | 20 | 0.12 |
| (1,3435) | 1:75:A:TRP:HH2 | 1:84:A:GLU:HA | 18 | 0.12 |
| (1,3431) | 1:73:A:GLN:HE22 | 1:125:A:TRP:HD1 | 1 | 0.12 |
| (1,3428) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HA | 5 | 0.12 |
| (1,3428) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HA | 11 | 0.12 |
| (1,3428) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HA | 20 | 0.12 |
| (1,3422) | 1:60:A:HIS:H | 1:75:A:TRP:HD1 | 1 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3419) | 1:75:A:TRP:HB2 | 1:75:A:TRP:HD1 | 5 | 0.12 |
| (1,3419) | 1:75:A:TRP:HB2 | 1:75:A:TRP:HD1 | 16 | 0.12 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD11 | 20 | 0.12 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD12 | 20 | 0.12 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD13 | 20 | 0.12 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD11 | 20 | 0.12 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD12 | 20 | 0.12 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD13 | 20 | 0.12 |
| (1,3402) | 1:26:A:PHE:H | 1:26:A:PHE:HD1 | 6 | 0.12 |
| (1,3402) | 1:26:A:PHE:H | 1:26:A:PHE:HD2 | 6 | 0.12 |
| (1,3402) | 1:26:A:PHE:H | 1:26:A:PHE:HD1 | 10 | 0.12 |
| (1,3402) | 1:26:A:PHE:H | 1:26:A:PHE:HD2 | 10 | 0.12 |
| (1,3396) | 1:25:A:PHE:HA | 1:26:A:PHE:HD1 | 6 | 0.12 |
| (1,3396) | 1:25:A:PHE:HA | 1:26:A:PHE:HD2 | 6 | 0.12 |
| (1,3395) | 1:26:A:PHE:HD1 | 1:59:A:TYR:H | 6 | 0.12 |
| (1,3395) | 1:26:A:PHE:HD2 | 1:59:A:TYR:H | 6 | 0.12 |
| (1,3387) | 1:87:A:ILE:HG21 | 1:111:A:PHE:HD1 | 17 | 0.12 |
| (1,3387) | 1:87:A:ILE:HG21 | 1:111:A:PHE:HD2 | 17 | 0.12 |
| (1,3387) | 1:87:A:ILE:HG22 | 1:111:A:PHE:HD1 | 17 | 0.12 |
| (1,3387) | 1:87:A:ILE:HG22 | 1:111:A:PHE:HD2 | 17 | 0.12 |
| (1,3387) | 1:87:A:ILE:HG23 | 1:111:A:PHE:HD1 | 17 | 0.12 |
| (1,3387) | 1:87:A:ILE:HG23 | 1:111:A:PHE:HD2 | 17 | 0.12 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD1 | 20 | 0.12 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD2 | 20 | 0.12 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD1 | 20 | 0.12 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD2 | 20 | 0.12 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD1 | 20 | 0.12 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD2 | 20 | 0.12 |
| (1,3371) | 1:167:A:THR:HG21 | 1:173:A:PHE:HD1 | 1 | 0.12 |
| (1,3371) | 1:167:A:THR:HG21 | 1:173:A:PHE:HD2 | 1 | 0.12 |
| (1,3371) | 1:167:A:THR:HG22 | 1:173:A:PHE:HD1 | 1 | 0.12 |
| (1,3371) | 1:167:A:THR:HG22 | 1:173:A:PHE:HD2 | 1 | 0.12 |
| (1,3371) | 1:167:A:THR:HG23 | 1:173:A:PHE:HD1 | 1 | 0.12 |
| (1,3371) | 1:167:A:THR:HG23 | 1:173:A:PHE:HD2 | 1 | 0.12 |
| (1,3363) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HA | 10 | 0.12 |
| (1,3363) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HA | 10 | 0.12 |
| (1,3363) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HA | 17 | 0.12 |
| (1,3363) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HA | 17 | 0.12 |
| (1,3359) | 1:167:A:THR:H | 1:173:A:PHE:HD1 | 10 | 0.12 |
| (1,3359) | 1:167:A:THR:H | 1:173:A:PHE:HD2 | 10 | 0.12 |
| (1,3350) | 1:153:A:TYR:HD1 | 1:160:A:LEU:H | 8 | 0.12 |
| (1,3350) | 1:153:A:TYR:HD2 | 1:160:A:LEU:H | 8 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD1 | 2 | 0.12 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD2 | 2 | 0.12 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD1 | 9 | 0.12 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD2 | 9 | 0.12 |
| (1,3336) | 1:92:A:PHE:HD1 | 1:96:A:GLN:HG2 | 4 | 0.12 |
| (1,3336) | 1:92:A:PHE:HD2 | 1:96:A:GLN:HG2 | 4 | 0.12 |
| (1,3336) | 1:92:A:PHE:HD1 | 1:96:A:GLN:HG2 | 16 | 0.12 |
| (1,3336) | 1:92:A:PHE:HD2 | 1:96:A:GLN:HG2 | 16 | 0.12 |
| (1,3336) | 1:92:A:PHE:HD1 | 1:96:A:GLN:HG2 | 17 | 0.12 |
| (1,3336) | 1:92:A:PHE:HD2 | 1:96:A:GLN:HG2 | 17 | 0.12 |
| (1,3325) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HD1 | 6 | 0.12 |
| (1,3325) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HD2 | 6 | 0.12 |
| (1,3325) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HD1 | 6 | 0.12 |
| (1,3325) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HD2 | 6 | 0.12 |
| (1,3325) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HD1 | 6 | 0.12 |
| (1,3325) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HD2 | 6 | 0.12 |
| (1,3325) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HD1 | 9 | 0.12 |
| (1,3325) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HD2 | 9 | 0.12 |
| (1,3325) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HD1 | 9 | 0.12 |
| (1,3325) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HD2 | 9 | 0.12 |
| (1,3325) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HD1 | 9 | 0.12 |
| (1,3325) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HD2 | 9 | 0.12 |
| (1,3305) | 1:38:A:GLU:H | 1:41:A:HIS:HE1 | 8 | 0.12 |
| (1,3274) | 1:118:A:GLY:HA3 | 1:121:A:TYR:H | 6 | 0.12 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD11 | 16 | 0.12 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD12 | 16 | 0.12 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD13 | 16 | 0.12 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG2 | 18 | 0.12 |
| (1,3172) | 1:89:A:ALA:HB1 | 1:90:A:PRO:HG3 | 18 | 0.12 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG2 | 18 | 0.12 |
| (1,3172) | 1:89:A:ALA:HB2 | 1:90:A:PRO:HG3 | 18 | 0.12 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG2 | 18 | 0.12 |
| (1,3172) | 1:89:A:ALA:HB3 | 1:90:A:PRO:HG3 | 18 | 0.12 |
| (1,3150) | 1:59:A:TYR:HA | 1:137:A:GLN:HG3 | 5 | 0.12 |
| (1,3132) | 1:24:A:GLU:HA | 1:152:A:MET:HE1 | 15 | 0.12 |
| (1,3132) | 1:24:A:GLU:HA | 1:152:A:MET:HE2 | 15 | 0.12 |
| (1,3132) | 1:24:A:GLU:HA | 1:152:A:MET:HE3 | 15 | 0.12 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD11 | 17 | 0.12 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD12 | 17 | 0.12 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD13 | 17 | 0.12 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD11 | 17 | 0.12 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD12 | 17 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD13 | 17 | 0.12 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD11 | 17 | 0.12 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD12 | 17 | 0.12 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD13 | 17 | 0.12 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB1 | 8 | 0.12 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB2 | 8 | 0.12 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB3 | 8 | 0.12 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB1 | 19 | 0.12 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB2 | 19 | 0.12 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB3 | 19 | 0.12 |
| (1,3082) | 1:24:A:GLU:HA | 1:25:A:PHE:HD1 | 3 | 0.12 |
| (1,3082) | 1:24:A:GLU:HA | 1:25:A:PHE:HD2 | 3 | 0.12 |
| (1,3061) | 1:49:A:LYS:HB3 | 1:178:A:ALA:HB1 | 3 | 0.12 |
| (1,3061) | 1:49:A:LYS:HB3 | 1:178:A:ALA:HB2 | 3 | 0.12 |
| (1,3061) | 1:49:A:LYS:HB3 | 1:178:A:ALA:HB3 | 3 | 0.12 |
| (1,3043) | 1:9:A:TYR:HD1 | 1:160:A:LEU:HA | 9 | 0.12 |
| (1,3043) | 1:9:A:TYR:HD2 | 1:160:A:LEU:HA | 9 | 0.12 |
| (1,3043) | 1:9:A:TYR:HD1 | 1:160:A:LEU:HA | 11 | 0.12 |
| (1,3043) | 1:9:A:TYR:HD2 | 1:160:A:LEU:HA | 11 | 0.12 |
| (1,3043) | 1:9:A:TYR:HD1 | 1:160:A:LEU:HA | 15 | 0.12 |
| (1,3043) | 1:9:A:TYR:HD2 | 1:160:A:LEU:HA | 15 | 0.12 |
| (1,3043) | 1:9:A:TYR:HD1 | 1:160:A:LEU:HA | 16 | 0.12 |
| (1,3043) | 1:9:A:TYR:HD2 | 1:160:A:LEU:HA | 16 | 0.12 |
| (1,3040) | 1:93:A:GLU:HG2 | 1:94:A:ALA:HA | 4 | 0.12 |
| (1,3040) | 1:93:A:GLU:HG3 | 1:94:A:ALA:HA | 4 | 0.12 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG11 | 10 | 0.12 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG12 | 10 | 0.12 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG13 | 10 | 0.12 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG11 | 13 | 0.12 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG12 | 13 | 0.12 |
| (1,3003) | 1:94:A:ALA:HA | 1:110:A:VAL:HG13 | 13 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB1 | 6 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB2 | 6 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB3 | 6 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB1 | 6 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB2 | 6 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB3 | 6 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB1 | 8 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB2 | 8 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB3 | 8 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB1 | 8 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB2 | 8 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB3 | 8 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB1 | 15 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB2 | 15 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB3 | 15 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB1 | 15 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB2 | 15 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB3 | 15 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB1 | 19 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB2 | 19 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB3 | 19 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB1 | 19 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB2 | 19 | 0.12 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB3 | 19 | 0.12 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB1 | 4 | 0.12 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB2 | 4 | 0.12 |
| (1,3000) | 1:23:A:LEU:HD11 | 1:140:A:ALA:HB3 | 4 | 0.12 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB1 | 4 | 0.12 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB2 | 4 | 0.12 |
| (1,3000) | 1:23:A:LEU:HD12 | 1:140:A:ALA:HB3 | 4 | 0.12 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB1 | 4 | 0.12 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB2 | 4 | 0.12 |
| (1,3000) | 1:23:A:LEU:HD13 | 1:140:A:ALA:HB3 | 4 | 0.12 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD11 | 11 | 0.12 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD12 | 11 | 0.12 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD13 | 11 | 0.12 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD21 | 11 | 0.12 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD22 | 11 | 0.12 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD23 | 11 | 0.12 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD11 | 15 | 0.12 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD12 | 15 | 0.12 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD13 | 15 | 0.12 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD21 | 15 | 0.12 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD22 | 15 | 0.12 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD23 | 15 | 0.12 |
| (1,2959) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HE1 | 16 | 0.12 |
| (1,2959) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HE2 | 16 | 0.12 |
| (1,2959) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HE1 | 16 | 0.12 |
| (1,2959) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HE2 | 16 | 0.12 |
| (1,2959) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HE1 | 16 | 0.12 |
| (1,2959) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HE2 | 16 | 0.12 |
| (1,2943) | 1:3:A:ILE:HG21 | 1:8:A:GLN:HG3 | 5 | 0.12 |
| (1,2943) | 1:3:A:ILE:HG22 | 1:8:A:GLN:HG3 | 5 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2943) | 1:3:A:ILE:HG23 | 1:8:A:GLN:HG3 | 5 | 0.12 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG11 | 19 | 0.12 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG12 | 19 | 0.12 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG13 | 19 | 0.12 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG11 | 19 | 0.12 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG12 | 19 | 0.12 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG13 | 19 | 0.12 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG11 | 19 | 0.12 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG12 | 19 | 0.12 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG13 | 19 | 0.12 |
| (1,2908) | 1:175:A:ALA:HA | 1:178:A:ALA:H | 7 | 0.12 |
| (1,2903) | 1:9:A:TYR:HA | 1:159:A:GLN:HA | 16 | 0.12 |
| (1,2889) | 1:74:A:ALA:HB1 | 1:107:A:ILE:HG21 | 11 | 0.12 |
| (1,2889) | 1:74:A:ALA:HB1 | 1:107:A:ILE:HG22 | 11 | 0.12 |
| (1,2889) | 1:74:A:ALA:HB1 | 1:107:A:ILE:HG23 | 11 | 0.12 |
| (1,2889) | 1:74:A:ALA:HB2 | 1:107:A:ILE:HG21 | 11 | 0.12 |
| (1,2889) | 1:74:A:ALA:HB2 | 1:107:A:ILE:HG22 | 11 | 0.12 |
| (1,2889) | 1:74:A:ALA:HB2 | 1:107:A:ILE:HG23 | 11 | 0.12 |
| (1,2889) | 1:74:A:ALA:HB3 | 1:107:A:ILE:HG21 | 11 | 0.12 |
| (1,2889) | 1:74:A:ALA:HB3 | 1:107:A:ILE:HG22 | 11 | 0.12 |
| (1,2889) | 1:74:A:ALA:HB3 | 1:107:A:ILE:HG23 | 11 | 0.12 |
| (1,2879) | 1:59:A:TYR:HE1 | 1:140:A:ALA:HA | 15 | 0.12 |
| (1,2879) | 1:59:A:TYR:HE2 | 1:140:A:ALA:HA | 15 | 0.12 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE1 | 20 | 0.12 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE2 | 20 | 0.12 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE3 | 20 | 0.12 |
| (1,2867) | 1:102:A:GLN:HA | 1:102:A:GLN:HB2 | 7 | 0.12 |
| (1,2865) | 1:17:A:ALA:H | 1:17:A:ALA:HB1 | 9 | 0.12 |
| (1,2865) | 1:17:A:ALA:H | 1:17:A:ALA:HB2 | 9 | 0.12 |
| (1,2865) | 1:17:A:ALA:H | 1:17:A:ALA:HB3 | 9 | 0.12 |
| (1,2849) | 1:26:A:PHE:H | 1:60:A:HIS:HA | 15 | 0.12 |
| (1,2847) | 1:2:A:GLN:HA | 1:2:A:GLN:HB3 | 15 | 0.12 |
| (1,2838) | 1:34:A:TYR:HE1 | 1:38:A:GLU:HA | 7 | 0.12 |
| (1,2838) | 1:34:A:TYR:HE2 | 1:38:A:GLU:HA | 7 | 0.12 |
| (1,2838) | 1:34:A:TYR:HE1 | 1:38:A:GLU:HA | 10 | 0.12 |
| (1,2838) | 1:34:A:TYR:HE2 | 1:38:A:GLU:HA | 10 | 0.12 |
| (1,2753) | 1:61:A:VAL:HG11 | 1:62:A:GLU:HA | 4 | 0.12 |
| (1,2753) | 1:61:A:VAL:HG12 | 1:62:A:GLU:HA | 4 | 0.12 |
| (1,2753) | 1:61:A:VAL:HG13 | 1:62:A:GLU:HA | 4 | 0.12 |
| (1,2742) | 1:77:A:VAL:HA | 1:130:A:VAL:HG11 | 11 | 0.12 |
| (1,2742) | 1:77:A:VAL:HA | 1:130:A:VAL:HG12 | 11 | 0.12 |
| (1,2742) | 1:77:A:VAL:HA | 1:130:A:VAL:HG13 | 11 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG11 | 4 | 0.12 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG12 | 4 | 0.12 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG13 | 4 | 0.12 |
| (1,2720) | 1:110:A:VAL:HA | 1:113:A:ASP:HA | 9 | 0.12 |
| (1,2714) | 1:104:A:VAL:HG11 | 1:106:A:ASP:H | 9 | 0.12 |
| (1,2714) | 1:104:A:VAL:HG12 | 1:106:A:ASP:H | 9 | 0.12 |
| (1,2714) | 1:104:A:VAL:HG13 | 1:106:A:ASP:H | 9 | 0.12 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG21 | 7 | 0.12 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG22 | 7 | 0.12 |
| (1,2673) | 1:180:A:THR:HA | 1:180:A:THR:HG23 | 7 | 0.12 |
| (1,2657) | 1:167:A:THR:HA | 1:167:A:THR:HG21 | 6 | 0.12 |
| (1,2657) | 1:167:A:THR:HA | 1:167:A:THR:HG22 | 6 | 0.12 |
| (1,2657) | 1:167:A:THR:HA | 1:167:A:THR:HG23 | 6 | 0.12 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 8 | 0.12 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 8 | 0.12 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 8 | 0.12 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 8 | 0.12 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 8 | 0.12 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 8 | 0.12 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 8 | 0.12 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 8 | 0.12 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 8 | 0.12 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG11 | 15 | 0.12 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG12 | 15 | 0.12 |
| (1,2576) | 1:100:A:THR:HG21 | 1:101:A:VAL:HG13 | 15 | 0.12 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG11 | 15 | 0.12 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG12 | 15 | 0.12 |
| (1,2576) | 1:100:A:THR:HG22 | 1:101:A:VAL:HG13 | 15 | 0.12 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG11 | 15 | 0.12 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG12 | 15 | 0.12 |
| (1,2576) | 1:100:A:THR:HG23 | 1:101:A:VAL:HG13 | 15 | 0.12 |
| (1,2487) | 1:8:A:GLN:HA | 1:161:A:ASN:HB2 | 7 | 0.12 |
| (1,2484) | 1:183:A:GLN:HA | 1:183:A:GLN:HB2 | 11 | 0.12 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 5 | 0.12 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 5 | 0.12 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 5 | 0.12 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 5 | 0.12 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 5 | 0.12 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 5 | 0.12 |
| (1,2417) | 1:73:A:GLN:HA | 1:77:A:VAL:HG21 | 18 | 0.12 |
| (1,2417) | 1:73:A:GLN:HA | 1:77:A:VAL:HG22 | 18 | 0.12 |
| (1,2417) | 1:73:A:GLN:HA | 1:77:A:VAL:HG23 | 18 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 11 | 0.12 |
| (1,2343) | 1:188:A:LYS:H | 1:188:A:LYS:HG2 | 8 | 0.12 |
| (1,2343) | 1:188:A:LYS:H | 1:188:A:LYS:HG3 | 8 | 0.12 |
| (1,2343) | 1:188:A:LYS:H | 1:188:A:LYS:HG2 | 18 | 0.12 |
| (1,2343) | 1:188:A:LYS:H | 1:188:A:LYS:HG3 | 18 | 0.12 |
| (1,2315) | 1:46:A:VAL:HG21 | 1:50:A:LEU:HG | 3 | 0.12 |
| (1,2315) | 1:46:A:VAL:HG22 | 1:50:A:LEU:HG | 3 | 0.12 |
| (1,2315) | 1:46:A:VAL:HG23 | 1:50:A:LEU:HG | 3 | 0.12 |
| (1,2315) | 1:46:A:VAL:HG21 | 1:50:A:LEU:HG | 5 | 0.12 |
| (1,2315) | 1:46:A:VAL:HG22 | 1:50:A:LEU:HG | 5 | 0.12 |
| (1,2315) | 1:46:A:VAL:HG23 | 1:50:A:LEU:HG | 5 | 0.12 |
| (1,2315) | 1:46:A:VAL:HG21 | 1:50:A:LEU:HG | 13 | 0.12 |
| (1,2315) | 1:46:A:VAL:HG22 | 1:50:A:LEU:HG | 13 | 0.12 |
| (1,2315) | 1:46:A:VAL:HG23 | 1:50:A:LEU:HG | 13 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 1 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 1 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 1 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 2 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 2 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 2 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 3 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 3 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 3 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 4 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 4 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 4 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 13 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 13 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 13 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 20 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 20 | 0.12 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 20 | 0.12 |
| (1,2253) | 1:77:A:VAL:HB | 1:125:A:TRP:HA | 9 | 0.12 |
| (1,2220) | 1:67:A:LEU:HD11 | 1:103:A:SER:HB2 | 4 | 0.12 |
| (1,2220) | 1:67:A:LEU:HD12 | 1:103:A:SER:HB2 | 4 | 0.12 |
| (1,2220) | 1:67:A:LEU:HD13 | 1:103:A:SER:HB2 | 4 | 0.12 |
| (1,2215) | 1:56:A:MET:HA | 1:57:A:THR:HA | 14 | 0.12 |
| (1,2194) | 1:98:A:THR:HA | 1:98:A:THR:HG21 | 10 | 0.12 |
| (1,2194) | 1:98:A:THR:HA | 1:98:A:THR:HG22 | 10 | 0.12 |
| (1,2194) | 1:98:A:THR:HA | 1:98:A:THR:HG23 | 10 | 0.12 |
| (1,2194) | 1:98:A:THR:HA | 1:98:A:THR:HG21 | 15 | 0.12 |
| (1,2194) | 1:98:A:THR:HA | 1:98:A:THR:HG22 | 15 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2194) | 1:98:A:THR:HA | 1:98:A:THR:HG23 | 15 | 0.12 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE1 | 2 | 0.12 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE2 | 2 | 0.12 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE3 | 2 | 0.12 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE1 | 2 | 0.12 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE2 | 2 | 0.12 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE3 | 2 | 0.12 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE1 | 6 | 0.12 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE2 | 6 | 0.12 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE3 | 6 | 0.12 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE1 | 6 | 0.12 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE2 | 6 | 0.12 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE3 | 6 | 0.12 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE1 | 9 | 0.12 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE2 | 9 | 0.12 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE3 | 9 | 0.12 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE1 | 9 | 0.12 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE2 | 9 | 0.12 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE3 | 9 | 0.12 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE1 | 19 | 0.12 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE2 | 19 | 0.12 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE3 | 19 | 0.12 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE1 | 19 | 0.12 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE2 | 19 | 0.12 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE3 | 19 | 0.12 |
| (1,2176) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HD2 | 15 | 0.12 |
| (1,2176) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HD3 | 15 | 0.12 |
| (1,2176) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HD2 | 15 | 0.12 |
| (1,2176) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HD3 | 15 | 0.12 |
| (1,2175) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HE2 | 17 | 0.12 |
| (1,2175) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HE3 | 17 | 0.12 |
| (1,2175) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HE2 | 17 | 0.12 |
| (1,2175) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HE3 | 17 | 0.12 |
| (1,2159) | 1:76:A:ALA:HA | 1:79:A:ILE:HG12 | 4 | 0.12 |
| (1,2158) | 1:87:A:ILE:HG12 | 1:88:A:THR:HA | 10 | 0.12 |
| (1,2157) | 1:39:A:VAL:H | 1:40:A:LEU:HG | 18 | 0.12 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD11 | 1 | 0.12 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD12 | 1 | 0.12 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD13 | 1 | 0.12 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD11 | 11 | 0.12 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD12 | 11 | 0.12 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD13 | 11 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD11 | 12 | 0.12 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD12 | 12 | 0.12 |
| (1,2133) | 1:29:A:TYR:HA | 1:71:A:LEU:HD13 | 12 | 0.12 |
| (1,2131) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HD22 | 18 | 0.12 |
| (1,2115) | 1:10:A:ILE:H | 1:10:A:ILE:HG13 | 20 | 0.12 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 15 | 0.12 |
| (1,1981) | 1:187:A:LYS:H | 1:187:A:LYS:HD3 | 17 | 0.12 |
| (1,1963) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HD2 | 1 | 0.12 |
| (1,1963) | 1:155:A:ASN:HB2 | 1:157:A:LYS:HD3 | 1 | 0.12 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 12 | 0.12 |
| (1,1937) | 1:75:A:TRP:HB2 | 1:78:A:ALA:H | 15 | 0.12 |
| (1,1916) | 1:91:A:MET:HB2 | 1:92:A:PHE:HE1 | 14 | 0.12 |
| (1,1916) | 1:91:A:MET:HB2 | 1:92:A:PHE:HE2 | 14 | 0.12 |
| (1,1915) | 1:186:A:GLU:HB2 | 1:187:A:LYS:H | 15 | 0.12 |
| (1,1878) | 1:60:A:HIS:HB2 | 1:72:A:THR:HG21 | 2 | 0.12 |
| (1,1878) | 1:60:A:HIS:HB2 | 1:72:A:THR:HG22 | 2 | 0.12 |
| (1,1878) | 1:60:A:HIS:HB2 | 1:72:A:THR:HG23 | 2 | 0.12 |
| (1,1873) | 1:46:A:VAL:HA | 1:49:A:LYS:HB3 | 19 | 0.12 |
| (1,1832) | 1:124:A:ALA:HB1 | 1:130:A:VAL:HB | 7 | 0.12 |
| (1,1832) | 1:124:A:ALA:HB2 | 1:130:A:VAL:HB | 7 | 0.12 |
| (1,1832) | 1:124:A:ALA:HB3 | 1:130:A:VAL:HB | 7 | 0.12 |
| (1,1832) | 1:124:A:ALA:HB1 | 1:130:A:VAL:HB | 14 | 0.12 |
| (1,1832) | 1:124:A:ALA:HB2 | 1:130:A:VAL:HB | 14 | 0.12 |
| (1,1832) | 1:124:A:ALA:HB3 | 1:130:A:VAL:HB | 14 | 0.12 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 2 | 0.12 |
| (1,1825) | 1:117:A:LYS:HB3 | 1:120:A:ASP:H | 13 | 0.12 |
| (1,1825) | 1:117:A:LYS:HB3 | 1:120:A:ASP:H | 19 | 0.12 |
| (1,1813) | 1:160:A:LEU:HD21 | 1:180:A:THR:HB | 17 | 0.12 |
| (1,1813) | 1:160:A:LEU:HD22 | 1:180:A:THR:HB | 17 | 0.12 |
| (1,1813) | 1:160:A:LEU:HD23 | 1:180:A:THR:HB | 17 | 0.12 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 2 | 0.12 |
| (1,1787) | 1:93:A:GLU:HA | 1:97:A:LYS:HB3 | 11 | 0.12 |
| (1,1785) | 1:97:A:LYS:HB2 | 1:97:A:LYS:HD2 | 8 | 0.12 |
| (1,1778) | 1:72:A:THR:HB | 1:73:A:GLN:HB3 | 18 | 0.12 |
| (1,1758) | 1:14:A:LYS:H | 1:14:A:LYS:HB3 | 12 | 0.12 |
| (1,1699) | 1:135:A:ALA:HB1 | 1:136:A:GLN:HG2 | 10 | 0.12 |
| (1,1699) | 1:135:A:ALA:HB2 | 1:136:A:GLN:HG2 | 10 | 0.12 |
| (1,1699) | 1:135:A:ALA:HB3 | 1:136:A:GLN:HG2 | 10 | 0.12 |
| (1,1693) | 1:136:A:GLN:H | 1:136:A:GLN:HG2 | 3 | 0.12 |
| (1,1693) | 1:136:A:GLN:H | 1:136:A:GLN:HG2 | 14 | 0.12 |
| (1,1676) | 1:163:A:GLN:H | 1:163:A:GLN:HG2 | 6 | 0.12 |
| (1,1676) | 1:163:A:GLN:H | 1:163:A:GLN:HG3 | 6 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1676) | 1:163:A:GLN:H | 1:163:A:GLN:HG2 | 8 | 0.12 |
| (1,1676) | 1:163:A:GLN:H | 1:163:A:GLN:HG3 | 8 | 0.12 |
| (1,1673) | 1:176:A:GLN:HG2 | 1:177:A:TYR:H | 12 | 0.12 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE1 | 16 | 0.12 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE2 | 16 | 0.12 |
| (1,1624) | 1:33:A:CYS:HA | 1:150:A:PRO:HB2 | 8 | 0.12 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB2 | 15 | 0.12 |
| (1,1615) | 1:26:A:PHE:H | 1:58:A:LYS:HB3 | 15 | 0.12 |
| (1,1513) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB2 | 4 | 0.12 |
| (1,1513) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB2 | 4 | 0.12 |
| (1,1513) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB2 | 4 | 0.12 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG11 | 5 | 0.12 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG12 | 5 | 0.12 |
| (1,1483) | 1:36:A:PHE:HB2 | 1:42:A:VAL:HG13 | 5 | 0.12 |
| (1,1450) | 1:42:A:VAL:HA | 1:45:A:ASN:HB3 | 9 | 0.12 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB2 | 6 | 0.12 |
| (1,1393) | 1:12:A:LEU:HA | 1:13:A:ASP:HB3 | 6 | 0.12 |
| (1,1298) | 1:141:A:ALA:HA | 1:146:A:LEU:HB2 | 3 | 0.12 |
| (1,1265) | 1:64:A:LEU:HB3 | 1:65:A:GLY:HA2 | 2 | 0.12 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 1 | 0.12 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 3 | 0.12 |
| (1,1080) | 1:34:A:TYR:HD1 | 1:38:A:GLU:H | 15 | 0.12 |
| (1,1055) | 1:94:A:ALA:HB1 | 1:96:A:GLN:H | 4 | 0.12 |
| (1,1055) | 1:94:A:ALA:HB2 | 1:96:A:GLN:H | 4 | 0.12 |
| (1,1055) | 1:94:A:ALA:HB3 | 1:96:A:GLN:H | 4 | 0.12 |
| (1,1040) | 1:52:A:GLU:HB3 | 1:53:A:GLY:H | 14 | 0.12 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 3 | 0.12 |
| (1,1011) | 1:169:A:ASN:HA | 1:169:A:ASN:HD22 | 9 | 0.12 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 1 | 0.12 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 2 | 0.12 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 2 | 0.12 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 3 | 0.12 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 3 | 0.12 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 5 | 0.12 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 5 | 0.12 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 6 | 0.12 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 6 | 0.12 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 8 | 0.12 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 8 | 0.12 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 9 | 0.12 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 9 | 0.12 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 11 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 11 | 0.12 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 12 | 0.12 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 12 | 0.12 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 16 | 0.12 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 16 | 0.12 |
| (1,938) | 1:112:A:VAL:HG11 | 1:118:A:GLY:H | 14 | 0.12 |
| (1,938) | 1:112:A:VAL:HG12 | 1:118:A:GLY:H | 14 | 0.12 |
| (1,938) | 1:112:A:VAL:HG13 | 1:118:A:GLY:H | 14 | 0.12 |
| (1,938) | 1:112:A:VAL:HG11 | 1:118:A:GLY:H | 16 | 0.12 |
| (1,938) | 1:112:A:VAL:HG12 | 1:118:A:GLY:H | 16 | 0.12 |
| (1,938) | 1:112:A:VAL:HG13 | 1:118:A:GLY:H | 16 | 0.12 |
| (1,936) | 1:117:A:LYS:HG3 | 1:118:A:GLY:H | 15 | 0.12 |
| (1,936) | 1:117:A:LYS:HG3 | 1:118:A:GLY:H | 16 | 0.12 |
| (1,909) | 1:126:A:ASN:HB3 | 1:127:A:SER:H | 8 | 0.12 |
| (1,815) | 1:91:A:MET:HB2 | 1:93:A:GLU:H | 16 | 0.12 |
| (1,815) | 1:91:A:MET:HB2 | 1:93:A:GLU:H | 17 | 0.12 |
| (1,809) | 1:179:A:ASP:HA | 1:180:A:THR:H | 1 | 0.12 |
| (1,809) | 1:179:A:ASP:HA | 1:180:A:THR:H | 12 | 0.12 |
| (1,799) | 1:49:A:LYS:HG2 | 1:179:A:ASP:H | 4 | 0.12 |
| (1,799) | 1:49:A:LYS:HG3 | 1:179:A:ASP:H | 4 | 0.12 |
| (1,747) | 1:118:A:GLY:HA2 | 1:119:A:GLU:H | 17 | 0.12 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 4 | 0.12 |
| (1,678) | 1:71:A:LEU:HD21 | 1:72:A:THR:H | 5 | 0.12 |
| (1,678) | 1:71:A:LEU:HD22 | 1:72:A:THR:H | 5 | 0.12 |
| (1,678) | 1:71:A:LEU:HD23 | 1:72:A:THR:H | 5 | 0.12 |
| (1,650) | 1:145:A:GLN:HA | 1:146:A:LEU:H | 13 | 0.12 |
| (1,632) | 1:87:A:ILE:HG21 | 1:91:A:MET:H | 6 | 0.12 |
| (1,632) | 1:87:A:ILE:HG22 | 1:91:A:MET:H | 6 | 0.12 |
| (1,632) | 1:87:A:ILE:HG23 | 1:91:A:MET:H | 6 | 0.12 |
| (1,568) | 1:49:A:LYS:HA | 1:50:A:LEU:H | 9 | 0.12 |
| (1,568) | 1:49:A:LYS:HA | 1:50:A:LEU:H | 12 | 0.12 |
| (1,568) | 1:49:A:LYS:HA | 1:50:A:LEU:H | 13 | 0.12 |
| (1,568) | 1:49:A:LYS:HA | 1:50:A:LEU:H | 19 | 0.12 |
| (1,553) | 1:42:A:VAL:HG21 | 1:46:A:VAL:H | 6 | 0.12 |
| (1,553) | 1:42:A:VAL:HG22 | 1:46:A:VAL:H | 6 | 0.12 |
| (1,553) | 1:42:A:VAL:HG23 | 1:46:A:VAL:H | 6 | 0.12 |
| (1,517) | 1:174:A:VAL:HG21 | 1:176:A:GLN:H | 19 | 0.12 |
| (1,517) | 1:174:A:VAL:HG22 | 1:176:A:GLN:H | 19 | 0.12 |
| (1,517) | 1:174:A:VAL:HG23 | 1:176:A:GLN:H | 19 | 0.12 |
| (1,456) | 1:60:A:HIS:HB3 | 1:75:A:TRP:H | 16 | 0.12 |
| (1,438) | 1:60:A:HIS:HB2 | 1:75:A:TRP:H | 13 | 0.12 |
| (1,353) | 1:108:A:ARG:HG3 | 1:112:A:VAL:H | 20 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,334) | 1:165:A:MET:HG2 | 1:166:A:ASP:H | 1 | 0.12 |
| (1,334) | 1:165:A:MET:HG3 | 1:166:A:ASP:H | 1 | 0.12 |
| (1,334) | 1:165:A:MET:HG2 | 1:166:A:ASP:H | 2 | 0.12 |
| (1,334) | 1:165:A:MET:HG3 | 1:166:A:ASP:H | 2 | 0.12 |
| (1,334) | 1:165:A:MET:HG2 | 1:166:A:ASP:H | 11 | 0.12 |
| (1,334) | 1:165:A:MET:HG3 | 1:166:A:ASP:H | 11 | 0.12 |
| (1,334) | 1:165:A:MET:HG2 | 1:166:A:ASP:H | 16 | 0.12 |
| (1,334) | 1:165:A:MET:HG3 | 1:166:A:ASP:H | 16 | 0.12 |
| (1,334) | 1:165:A:MET:HG2 | 1:166:A:ASP:H | 20 | 0.12 |
| (1,334) | 1:165:A:MET:HG3 | 1:166:A:ASP:H | 20 | 0.12 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 18 | 0.12 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 18 | 0.12 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 18 | 0.12 |
| (1,300) | 1:130:A:VAL:HG21 | 1:131:A:LYS:H | 8 | 0.12 |
| (1,300) | 1:130:A:VAL:HG22 | 1:131:A:LYS:H | 8 | 0.12 |
| (1,300) | 1:130:A:VAL:HG23 | 1:131:A:LYS:H | 8 | 0.12 |
| (1,300) | 1:130:A:VAL:HG21 | 1:131:A:LYS:H | 9 | 0.12 |
| (1,300) | 1:130:A:VAL:HG22 | 1:131:A:LYS:H | 9 | 0.12 |
| (1,300) | 1:130:A:VAL:HG23 | 1:131:A:LYS:H | 9 | 0.12 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 1 | 0.12 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 1 | 0.12 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 2 | 0.12 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 2 | 0.12 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 4 | 0.12 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 4 | 0.12 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 16 | 0.12 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 16 | 0.12 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 19 | 0.12 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 19 | 0.12 |
| (1,259) | 1:69:A:LYS:HD2 | 1:70:A:ASP:H | 3 | 0.12 |
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 14 | 0.12 |
| (1,241) | 1:70:A:ASP:HB2 | 1:74:A:ALA:H | 10 | 0.12 |
| (1,235) | 1:87:A:ILE:HG21 | 1:89:A:ALA:H | 8 | 0.12 |
| (1,235) | 1:87:A:ILE:HG22 | 1:89:A:ALA:H | 8 | 0.12 |
| (1,235) | 1:87:A:ILE:HG23 | 1:89:A:ALA:H | 8 | 0.12 |
| (1,216) | 1:34:A:TYR:H | 1:96:A:GLN:HE21 | 16 | 0.12 |
| (1,193) | 1:25:A:PHE:HB2 | 1:151:A:ALA:H | 15 | 0.12 |
| (1,193) | 1:25:A:PHE:HB3 | 1:151:A:ALA:H | 15 | 0.12 |
| (1,184) | 1:60:A:HIS:H | 1:72:A:THR:HA | 5 | 0.12 |
| (1,184) | 1:60:A:HIS:H | 1:72:A:THR:HA | 9 | 0.12 |
| (1,184) | 1:60:A:HIS:H | 1:72:A:THR:HA | 15 | 0.12 |
| (1,175) | 1:87:A:ILE:HG21 | 1:113:A:ASP:H | 3 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,175) | 1:87:A:ILE:HG22 | 1:113:A:ASP:H | 3 | 0.12 |
| (1,175) | 1:87:A:ILE:HG23 | 1:113:A:ASP:H | 3 | 0.12 |
| (1,175) | 1:87:A:ILE:HG21 | 1:113:A:ASP:H | 5 | 0.12 |
| (1,175) | 1:87:A:ILE:HG22 | 1:113:A:ASP:H | 5 | 0.12 |
| (1,175) | 1:87:A:ILE:HG23 | 1:113:A:ASP:H | 5 | 0.12 |
| (1,175) | 1:87:A:ILE:HG21 | 1:113:A:ASP:H | 9 | 0.12 |
| (1,175) | 1:87:A:ILE:HG22 | 1:113:A:ASP:H | 9 | 0.12 |
| (1,175) | 1:87:A:ILE:HG23 | 1:113:A:ASP:H | 9 | 0.12 |
| (1,175) | 1:87:A:ILE:HG21 | 1:113:A:ASP:H | 20 | 0.12 |
| (1,175) | 1:87:A:ILE:HG22 | 1:113:A:ASP:H | 20 | 0.12 |
| (1,175) | 1:87:A:ILE:HG23 | 1:113:A:ASP:H | 20 | 0.12 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD21 | 3 | 0.12 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD22 | 3 | 0.12 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD23 | 3 | 0.12 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD21 | 4 | 0.12 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD22 | 4 | 0.12 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD23 | 4 | 0.12 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD21 | 7 | 0.12 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD22 | 7 | 0.12 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD23 | 7 | 0.12 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD21 | 19 | 0.12 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD22 | 19 | 0.12 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD23 | 19 | 0.12 |
| (1,138) | 1:80:A:ALA:H | 1:81:A:LEU:HA | 9 | 0.12 |
| (1,138) | 1:80:A:ALA:H | 1:81:A:LEU:HA | 19 | 0.12 |
| (1,126) | 1:10:A:ILE:HG21 | 1:159:A:GLN:H | 16 | 0.12 |
| (1,126) | 1:10:A:ILE:HG22 | 1:159:A:GLN:H | 16 | 0.12 |
| (1,126) | 1:10:A:ILE:HG23 | 1:159:A:GLN:H | 16 | 0.12 |
| (1,126) | 1:10:A:ILE:HG21 | 1:159:A:GLN:H | 18 | 0.12 |
| (1,126) | 1:10:A:ILE:HG22 | 1:159:A:GLN:H | 18 | 0.12 |
| (1,126) | 1:10:A:ILE:HG23 | 1:159:A:GLN:H | 18 | 0.12 |
| (1,28) | 1:58:A:LYS:HG2 | 1:75:A:TRP:HE1 | 4 | 0.12 |
| (1,28) | 1:58:A:LYS:HG3 | 1:75:A:TRP:HE1 | 4 | 0.12 |
| (1,28) | 1:58:A:LYS:HG2 | 1:75:A:TRP:HE1 | 15 | 0.12 |
| (1,28) | 1:58:A:LYS:HG3 | 1:75:A:TRP:HE1 | 15 | 0.12 |
| (1,12) | 1:16:A:ILE:HD11 | 1:17:A:ALA:H | 20 | 0.12 |
| (1,12) | 1:16:A:ILE:HD12 | 1:17:A:ALA:H | 20 | 0.12 |
| (1,12) | 1:16:A:ILE:HD13 | 1:17:A:ALA:H | 20 | 0.12 |
| (1,3531) | 1:58:A:LYS:H | 1:75:A:TRP:HZ2 | 20 | 0.11 |
| (1,3524) | 1:70:A:ASP:HA | 1:125:A:TRP:HZ2 | 13 | 0.11 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE1 | 3 | 0.11 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE2 | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE1 | 20 | 0.11 |
| (1,3513) | 1:160:A:LEU:HA | 1:177:A:TYR:HE2 | 20 | 0.11 |
| (1,3508) | 1:34:A:TYR:HE1 | 1:97:A:LYS:H | 13 | 0.11 |
| (1,3508) | 1:34:A:TYR:HE2 | 1:97:A:LYS:H | 13 | 0.11 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE1 | 4 | 0.11 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE2 | 4 | 0.11 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE1 | 19 | 0.11 |
| (1,3482) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HE2 | 19 | 0.11 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE1 | 19 | 0.11 |
| (1,3482) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HE2 | 19 | 0.11 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE1 | 19 | 0.11 |
| (1,3482) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HE2 | 19 | 0.11 |
| (1,3477) | 1:32:A:HIS:HA | 1:32:A:HIS:HD2 | 12 | 0.11 |
| (1,3470) | 1:77:A:VAL:HB | 1:125:A:TRP:HE3 | 11 | 0.11 |
| (1,3465) | 1:74:A:ALA:HB1 | 1:125:A:TRP:HE3 | 2 | 0.11 |
| (1,3465) | 1:74:A:ALA:HB2 | 1:125:A:TRP:HE3 | 2 | 0.11 |
| (1,3465) | 1:74:A:ALA:HB3 | 1:125:A:TRP:HE3 | 2 | 0.11 |
| (1,3463) | 1:77:A:VAL:H | 1:125:A:TRP:HE3 | 3 | 0.11 |
| (1,3461) | 1:75:A:TRP:HB3 | 1:75:A:TRP:HE3 | 1 | 0.11 |
| (1,3461) | 1:75:A:TRP:HB3 | 1:75:A:TRP:HE3 | 19 | 0.11 |
| (1,3458) | 1:38:A:GLU:HA | 1:41:A:HIS:HD2 | 8 | 0.11 |
| (1,3445) | 1:75:A:TRP:HZ3 | 1:84:A:GLU:HG3 | 11 | 0.11 |
| (1,3431) | 1:73:A:GLN:HE22 | 1:125:A:TRP:HD1 | 9 | 0.11 |
| (1,3428) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HA | 1 | 0.11 |
| (1,3428) | 1:125:A:TRP:HD1 | 1:126:A:ASN:HA | 15 | 0.11 |
| (1,3422) | 1:60:A:HIS:H | 1:75:A:TRP:HD1 | 11 | 0.11 |
| (1,3419) | 1:75:A:TRP:HB2 | 1:75:A:TRP:HD1 | 1 | 0.11 |
| (1,3419) | 1:75:A:TRP:HB2 | 1:75:A:TRP:HD1 | 2 | 0.11 |
| (1,3419) | 1:75:A:TRP:HB2 | 1:75:A:TRP:HD1 | 15 | 0.11 |
| (1,3404) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HB2 | 3 | 0.11 |
| (1,3404) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HB3 | 3 | 0.11 |
| (1,3404) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HB2 | 3 | 0.11 |
| (1,3404) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HB3 | 3 | 0.11 |
| (1,3388) | 1:34:A:TYR:HD1 | 1:92:A:PHE:HA | 5 | 0.11 |
| (1,3388) | 1:34:A:TYR:HD2 | 1:92:A:PHE:HA | 5 | 0.11 |
| (1,3388) | 1:34:A:TYR:HD1 | 1:92:A:PHE:HA | 18 | 0.11 |
| (1,3388) | 1:34:A:TYR:HD2 | 1:92:A:PHE:HA | 18 | 0.11 |
| (1,3388) | 1:34:A:TYR:HD1 | 1:92:A:PHE:HA | 19 | 0.11 |
| (1,3388) | 1:34:A:TYR:HD2 | 1:92:A:PHE:HA | 19 | 0.11 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD1 | 2 | 0.11 |
| (1,3373) | 1:151:A:ALA:HB1 | 1:153:A:TYR:HD2 | 2 | 0.11 |
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD1 | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3373) | 1:151:A:ALA:HB2 | 1:153:A:TYR:HD2 | 2 | 0.11 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD1 | 2 | 0.11 |
| (1,3373) | 1:151:A:ALA:HB3 | 1:153:A:TYR:HD2 | 2 | 0.11 |
| (1,3363) | 1:153:A:TYR:HD1 | 1:159:A:GLN:HA | 14 | 0.11 |
| (1,3363) | 1:153:A:TYR:HD2 | 1:159:A:GLN:HA | 14 | 0.11 |
| (1,3356) | 1:25:A:PHE:H | 1:25:A:PHE:HD1 | 17 | 0.11 |
| (1,3356) | 1:25:A:PHE:H | 1:25:A:PHE:HD2 | 17 | 0.11 |
| (1,3349) | 1:25:A:PHE:HD1 | 1:151:A:ALA:HB1 | 2 | 0.11 |
| (1,3349) | 1:25:A:PHE:HD1 | 1:151:A:ALA:HB2 | 2 | 0.11 |
| (1,3349) | 1:25:A:PHE:HD1 | 1:151:A:ALA:HB3 | 2 | 0.11 |
| (1,3349) | 1:25:A:PHE:HD2 | 1:151:A:ALA:HB1 | 2 | 0.11 |
| (1,3349) | 1:25:A:PHE:HD2 | 1:151:A:ALA:HB2 | 2 | 0.11 |
| (1,3349) | 1:25:A:PHE:HD2 | 1:151:A:ALA:HB3 | 2 | 0.11 |
| (1,3348) | 1:63:A:PHE:HA | 1:63:A:PHE:HD1 | 20 | 0.11 |
| (1,3348) | 1:63:A:PHE:HA | 1:63:A:PHE:HD2 | 20 | 0.11 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD1 | 1 | 0.11 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD2 | 1 | 0.11 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD1 | 5 | 0.11 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD2 | 5 | 0.11 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD1 | 17 | 0.11 |
| (1,3339) | 1:177:A:TYR:H | 1:177:A:TYR:HD2 | 17 | 0.11 |
| (1,3331) | 1:91:A:MET:H | 1:92:A:PHE:HD1 | 14 | 0.11 |
| (1,3331) | 1:91:A:MET:H | 1:92:A:PHE:HD2 | 14 | 0.11 |
| (1,3325) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HD1 | 17 | 0.11 |
| (1,3325) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HD2 | 17 | 0.11 |
| (1,3325) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HD1 | 17 | 0.11 |
| (1,3325) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HD2 | 17 | 0.11 |
| (1,3325) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HD1 | 17 | 0.11 |
| (1,3325) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HD2 | 17 | 0.11 |
| (1,3306) | 1:38:A:GLU:HA | 1:41:A:HIS:HE1 | 6 | 0.11 |
| (1,3269) | 1:112:A:VAL:HG11 | 1:118:A:GLY:HA2 | 19 | 0.11 |
| (1,3269) | 1:112:A:VAL:HG12 | 1:118:A:GLY:HA2 | 19 | 0.11 |
| (1,3269) | 1:112:A:VAL:HG13 | 1:118:A:GLY:HA2 | 19 | 0.11 |
| (1,3260) | 1:10:A:ILE:HD11 | 1:11:A:THR:H | 18 | 0.11 |
| (1,3260) | 1:10:A:ILE:HD12 | 1:11:A:THR:H | 18 | 0.11 |
| (1,3260) | 1:10:A:ILE:HD13 | 1:11:A:THR:H | 18 | 0.11 |
| (1,3252) | 1:29:A:TYR:HD1 | 1:68:A:GLY:HA3 | 2 | 0.11 |
| (1,3252) | 1:29:A:TYR:HD2 | 1:68:A:GLY:HA3 | 2 | 0.11 |
| (1,3212) | 1:87:A:ILE:HD11 | 1:91:A:MET:HG2 | 6 | 0.11 |
| (1,3212) | 1:87:A:ILE:HD11 | 1:91:A:MET:HG3 | 6 | 0.11 |
| (1,3212) | 1:87:A:ILE:HD12 | 1:91:A:MET:HG2 | 6 | 0.11 |
| (1,3212) | 1:87:A:ILE:HD12 | 1:91:A:MET:HG3 | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3212) | 1:87:A:ILE:HD13 | 1:91:A:MET:HG2 | 6 | 0.11 |
| (1,3212) | 1:87:A:ILE:HD13 | 1:91:A:MET:HG3 | 6 | 0.11 |
| (1,3199) | 1:3:A:ILE:HD11 | 1:184:A:LEU:HA | 18 | 0.11 |
| (1,3199) | 1:3:A:ILE:HD12 | 1:184:A:LEU:HA | 18 | 0.11 |
| (1,3199) | 1:3:A:ILE:HD13 | 1:184:A:LEU:HA | 18 | 0.11 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD11 | 1 | 0.11 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD12 | 1 | 0.11 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD13 | 1 | 0.11 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD11 | 6 | 0.11 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD12 | 6 | 0.11 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD13 | 6 | 0.11 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD11 | 20 | 0.11 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD12 | 20 | 0.11 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD13 | 20 | 0.11 |
| (1,3169) | 1:88:A:THR:H | 1:89:A:ALA:HB1 | 5 | 0.11 |
| (1,3169) | 1:88:A:THR:H | 1:89:A:ALA:HB2 | 5 | 0.11 |
| (1,3169) | 1:88:A:THR:H | 1:89:A:ALA:HB3 | 5 | 0.11 |
| (1,3137) | 1:25:A:PHE:H | 1:152:A:MET:HE1 | 10 | 0.11 |
| (1,3137) | 1:25:A:PHE:H | 1:152:A:MET:HE2 | 10 | 0.11 |
| (1,3137) | 1:25:A:PHE:H | 1:152:A:MET:HE3 | 10 | 0.11 |
| (1,3132) | 1:24:A:GLU:HA | 1:152:A:MET:HE1 | 3 | 0.11 |
| (1,3132) | 1:24:A:GLU:HA | 1:152:A:MET:HE2 | 3 | 0.11 |
| (1,3132) | 1:24:A:GLU:HA | 1:152:A:MET:HE3 | 3 | 0.11 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD11 | 4 | 0.11 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD12 | 4 | 0.11 |
| (1,3131) | 1:152:A:MET:HE1 | 1:160:A:LEU:HD13 | 4 | 0.11 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD11 | 4 | 0.11 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD12 | 4 | 0.11 |
| (1,3131) | 1:152:A:MET:HE2 | 1:160:A:LEU:HD13 | 4 | 0.11 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD11 | 4 | 0.11 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD12 | 4 | 0.11 |
| (1,3131) | 1:152:A:MET:HE3 | 1:160:A:LEU:HD13 | 4 | 0.11 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB1 | 1 | 0.11 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB2 | 1 | 0.11 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB3 | 1 | 0.11 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB1 | 9 | 0.11 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB2 | 9 | 0.11 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB3 | 9 | 0.11 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB1 | 10 | 0.11 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB2 | 10 | 0.11 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB3 | 10 | 0.11 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB1 | 12 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB2 | 12 | 0.11 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB3 | 12 | 0.11 |
| (1,3076) | 1:47:A:ARG:HG3 | 1:56:A:MET:HE1 | 4 | 0.11 |
| (1,3076) | 1:47:A:ARG:HG3 | 1:56:A:MET:HE2 | 4 | 0.11 |
| (1,3076) | 1:47:A:ARG:HG3 | 1:56:A:MET:HE3 | 4 | 0.11 |
| (1,3076) | 1:47:A:ARG:HG3 | 1:56:A:MET:HE1 | 13 | 0.11 |
| (1,3076) | 1:47:A:ARG:HG3 | 1:56:A:MET:HE2 | 13 | 0.11 |
| (1,3076) | 1:47:A:ARG:HG3 | 1:56:A:MET:HE3 | 13 | 0.11 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG21 | 20 | 0.11 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG22 | 20 | 0.11 |
| (1,3069) | 1:91:A:MET:HE1 | 1:110:A:VAL:HG23 | 20 | 0.11 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG21 | 20 | 0.11 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG22 | 20 | 0.11 |
| (1,3069) | 1:91:A:MET:HE2 | 1:110:A:VAL:HG23 | 20 | 0.11 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG21 | 20 | 0.11 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG22 | 20 | 0.11 |
| (1,3069) | 1:91:A:MET:HE3 | 1:110:A:VAL:HG23 | 20 | 0.11 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB1 | 11 | 0.11 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB2 | 11 | 0.11 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB3 | 11 | 0.11 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB1 | 11 | 0.11 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB2 | 11 | 0.11 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB3 | 11 | 0.11 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB1 | 11 | 0.11 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB2 | 11 | 0.11 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB3 | 11 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG2 | 1:178:A:ALA:HB1 | 13 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG2 | 1:178:A:ALA:HB2 | 13 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG2 | 1:178:A:ALA:HB3 | 13 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG3 | 1:178:A:ALA:HB1 | 13 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG3 | 1:178:A:ALA:HB2 | 13 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG3 | 1:178:A:ALA:HB3 | 13 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG2 | 1:178:A:ALA:HB1 | 19 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG2 | 1:178:A:ALA:HB2 | 19 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG2 | 1:178:A:ALA:HB3 | 19 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG3 | 1:178:A:ALA:HB1 | 19 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG3 | 1:178:A:ALA:HB2 | 19 | 0.11 |
| (1,3062) | 1:49:A:LYS:HG3 | 1:178:A:ALA:HB3 | 19 | 0.11 |
| (1,3043) | 1:9:A:TYR:HD1 | 1:160:A:LEU:HA | 2 | 0.11 |
| (1,3043) | 1:9:A:TYR:HD2 | 1:160:A:LEU:HA | 2 | 0.11 |
| (1,3043) | 1:9:A:TYR:HD1 | 1:160:A:LEU:HA | 3 | 0.11 |
| (1,3043) | 1:9:A:TYR:HD2 | 1:160:A:LEU:HA | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3043) | 1:9:A:TYR:HD1 | 1:160:A:LEU:HA | 4 | 0.11 |
| (1,3043) | 1:9:A:TYR:HD2 | 1:160:A:LEU:HA | 4 | 0.11 |
| (1,3043) | 1:9:A:TYR:HD1 | 1:160:A:LEU:HA | 6 | 0.11 |
| (1,3043) | 1:9:A:TYR:HD2 | 1:160:A:LEU:HA | 6 | 0.11 |
| (1,3043) | 1:9:A:TYR:HD1 | 1:160:A:LEU:HA | 10 | 0.11 |
| (1,3043) | 1:9:A:TYR:HD2 | 1:160:A:LEU:HA | 10 | 0.11 |
| (1,3043) | 1:9:A:TYR:HD1 | 1:160:A:LEU:HA | 12 | 0.11 |
| (1,3043) | 1:9:A:TYR:HD2 | 1:160:A:LEU:HA | 12 | 0.11 |
| (1,3043) | 1:9:A:TYR:HD1 | 1:160:A:LEU:HA | 17 | 0.11 |
| (1,3043) | 1:9:A:TYR:HD2 | 1:160:A:LEU:HA | 17 | 0.11 |
| (1,3015) | 1:167:A:THR:HA | 1:170:A:MET:HE1 | 10 | 0.11 |
| (1,3015) | 1:167:A:THR:HA | 1:170:A:MET:HE2 | 10 | 0.11 |
| (1,3015) | 1:167:A:THR:HA | 1:170:A:MET:HE3 | 10 | 0.11 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD21 | 6 | 0.11 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD22 | 6 | 0.11 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD23 | 6 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB1 | 5 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB2 | 5 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB3 | 5 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB1 | 5 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB2 | 5 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB3 | 5 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB1 | 10 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB2 | 10 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB3 | 10 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB1 | 10 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB2 | 10 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB3 | 10 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB1 | 14 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB2 | 14 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB3 | 14 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB1 | 14 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB2 | 14 | 0.11 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB3 | 14 | 0.11 |
| (1,2996) | 1:140:A:ALA:HB1 | 1:141:A:ALA:H | 9 | 0.11 |
| (1,2996) | 1:140:A:ALA:HB2 | 1:141:A:ALA:H | 9 | 0.11 |
| (1,2996) | 1:140:A:ALA:HB3 | 1:141:A:ALA:H | 9 | 0.11 |
| (1,2996) | 1:140:A:ALA:HB1 | 1:141:A:ALA:H | 12 | 0.11 |
| (1,2996) | 1:140:A:ALA:HB2 | 1:141:A:ALA:H | 12 | 0.11 |
| (1,2996) | 1:140:A:ALA:HB3 | 1:141:A:ALA:H | 12 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB1 | 9 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB2 | 9 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB3 | 9 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB1 | 9 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB2 | 9 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB3 | 9 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB1 | 12 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB2 | 12 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB3 | 12 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB1 | 12 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB2 | 12 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB3 | 12 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB1 | 19 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB2 | 19 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB3 | 19 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB1 | 19 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB2 | 19 | 0.11 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB3 | 19 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD11 | 3 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD12 | 3 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD13 | 3 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD21 | 3 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD22 | 3 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD23 | 3 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD11 | 6 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD12 | 6 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD13 | 6 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD21 | 6 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD22 | 6 | 0.11 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD23 | 6 | 0.11 |
| (1,2968) | 1:123:A:ALA:HA | 1:126:A:ASN:HB2 | 7 | 0.11 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG11 | 2 | 0.11 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG12 | 2 | 0.11 |
| (1,2958) | 1:27:A:SER:HA | 1:61:A:VAL:HG13 | 2 | 0.11 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG11 | 16 | 0.11 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG12 | 16 | 0.11 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG13 | 16 | 0.11 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG11 | 16 | 0.11 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG12 | 16 | 0.11 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG13 | 16 | 0.11 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG11 | 16 | 0.11 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG12 | 16 | 0.11 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG13 | 16 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD21 | 1:74:A:ALA:HB1 | 13 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2890) | 1:71:A:LEU:HD21 | 1:74:A:ALA:HB2 | 13 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD21 | 1:74:A:ALA:HB3 | 13 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD22 | 1:74:A:ALA:HB1 | 13 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD22 | 1:74:A:ALA:HB2 | 13 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD22 | 1:74:A:ALA:HB3 | 13 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD23 | 1:74:A:ALA:HB1 | 13 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD23 | 1:74:A:ALA:HB2 | 13 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD23 | 1:74:A:ALA:HB3 | 13 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD21 | 1:74:A:ALA:HB1 | 15 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD21 | 1:74:A:ALA:HB2 | 15 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD21 | 1:74:A:ALA:HB3 | 15 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD22 | 1:74:A:ALA:HB1 | 15 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD22 | 1:74:A:ALA:HB2 | 15 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD22 | 1:74:A:ALA:HB3 | 15 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD23 | 1:74:A:ALA:HB1 | 15 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD23 | 1:74:A:ALA:HB2 | 15 | 0.11 |
| (1,2890) | 1:71:A:LEU:HD23 | 1:74:A:ALA:HB3 | 15 | 0.11 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE1 | 5 | 0.11 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE2 | 5 | 0.11 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE3 | 5 | 0.11 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE1 | 9 | 0.11 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE2 | 9 | 0.11 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE3 | 9 | 0.11 |
| (1,2830) | 1:25:A:PHE:HA | 1:149:A:VAL:HG11 | 13 | 0.11 |
| (1,2830) | 1:25:A:PHE:HA | 1:149:A:VAL:HG12 | 13 | 0.11 |
| (1,2830) | 1:25:A:PHE:HA | 1:149:A:VAL:HG13 | 13 | 0.11 |
| (1,2830) | 1:25:A:PHE:HA | 1:149:A:VAL:HG21 | 13 | 0.11 |
| (1,2830) | 1:25:A:PHE:HA | 1:149:A:VAL:HG22 | 13 | 0.11 |
| (1,2830) | 1:25:A:PHE:HA | 1:149:A:VAL:HG23 | 13 | 0.11 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD11 | 7 | 0.11 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD12 | 7 | 0.11 |
| (1,2814) | 1:85:A:ASP:HA | 1:87:A:ILE:HD13 | 7 | 0.11 |
| (1,2787) | 1:86:A:LYS:H | 1:87:A:ILE:HG21 | 20 | 0.11 |
| (1,2787) | 1:86:A:LYS:H | 1:87:A:ILE:HG22 | 20 | 0.11 |
| (1,2787) | 1:86:A:LYS:H | 1:87:A:ILE:HG23 | 20 | 0.11 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD21 | 14 | 0.11 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD22 | 14 | 0.11 |
| (1,2760) | 1:146:A:LEU:HA | 1:146:A:LEU:HD23 | 14 | 0.11 |
| (1,2742) | 1:77:A:VAL:HA | 1:130:A:VAL:HG11 | 8 | 0.11 |
| (1,2742) | 1:77:A:VAL:HA | 1:130:A:VAL:HG12 | 8 | 0.11 |
| (1,2742) | 1:77:A:VAL:HA | 1:130:A:VAL:HG13 | 8 | 0.11 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG11 | 11 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG12 | 11 | 0.11 |
| (1,2733) | 1:35:A:GLN:HG2 | 1:39:A:VAL:HG13 | 11 | 0.11 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG11 | 11 | 0.11 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG12 | 11 | 0.11 |
| (1,2733) | 1:35:A:GLN:HG3 | 1:39:A:VAL:HG13 | 11 | 0.11 |
| (1,2724) | 1:124:A:ALA:HA | 1:130:A:VAL:HG11 | 3 | 0.11 |
| (1,2724) | 1:124:A:ALA:HA | 1:130:A:VAL:HG12 | 3 | 0.11 |
| (1,2724) | 1:124:A:ALA:HA | 1:130:A:VAL:HG13 | 3 | 0.11 |
| (1,2713) | 1:104:A:VAL:HG11 | 1:105:A:ALA:H | 8 | 0.11 |
| (1,2713) | 1:104:A:VAL:HG12 | 1:105:A:ALA:H | 8 | 0.11 |
| (1,2713) | 1:104:A:VAL:HG13 | 1:105:A:ALA:H | 8 | 0.11 |
| (1,2678) | 1:9:A:TYR:H | 1:180:A:THR:HG21 | 16 | 0.11 |
| (1,2678) | 1:9:A:TYR:H | 1:180:A:THR:HG22 | 16 | 0.11 |
| (1,2678) | 1:9:A:TYR:H | 1:180:A:THR:HG23 | 16 | 0.11 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG11 | 13 | 0.11 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG12 | 13 | 0.11 |
| (1,2660) | 1:95:A:VAL:H | 1:101:A:VAL:HG13 | 13 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD11 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD12 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD13 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD21 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD22 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB1 | 1:81:A:LEU:HD23 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD11 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD12 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD13 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD21 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD22 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB2 | 1:81:A:LEU:HD23 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD11 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD12 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD13 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD21 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD22 | 4 | 0.11 |
| (1,2659) | 1:80:A:ALA:HB3 | 1:81:A:LEU:HD23 | 4 | 0.11 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG21 | 10 | 0.11 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG22 | 10 | 0.11 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG23 | 10 | 0.11 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG21 | 10 | 0.11 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG22 | 10 | 0.11 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG23 | 10 | 0.11 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG21 | 10 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG22 | 10 | 0.11 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG23 | 10 | 0.11 |
| (1,2653) | 1:38:A:GLU:HG2 | 1:88:A:THR:HG21 | 10 | 0.11 |
| (1,2653) | 1:38:A:GLU:HG2 | 1:88:A:THR:HG22 | 10 | 0.11 |
| (1,2653) | 1:38:A:GLU:HG2 | 1:88:A:THR:HG23 | 10 | 0.11 |
| (1,2640) | 1:170:A:MET:HA | 1:171:A:ASP:H | 1 | 0.11 |
| (1,2622) | 1:149:A:VAL:HA | 1:151:A:ALA:H | 9 | 0.11 |
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 1 | 0.11 |
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 3 | 0.11 |
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 4 | 0.11 |
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 6 | 0.11 |
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 8 | 0.11 |
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 9 | 0.11 |
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 10 | 0.11 |
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 11 | 0.11 |
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 12 | 0.11 |
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 14 | 0.11 |
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 15 | 0.11 |
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 17 | 0.11 |
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 19 | 0.11 |
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 20 | 0.11 |
| (1,2596) | 1:63:A:PHE:HA | 1:64:A:LEU:H | 2 | 0.11 |
| (1,2586) | 1:188:A:LYS:HA | 1:188:A:LYS:HG2 | 11 | 0.11 |
| (1,2586) | 1:188:A:LYS:HA | 1:188:A:LYS:HG3 | 11 | 0.11 |
| (1,2586) | 1:188:A:LYS:HA | 1:188:A:LYS:HG2 | 15 | 0.11 |
| (1,2586) | 1:188:A:LYS:HA | 1:188:A:LYS:HG3 | 15 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG21 | 5 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG22 | 5 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG23 | 5 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG21 | 5 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG22 | 5 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG23 | 5 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG21 | 5 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG22 | 5 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG23 | 5 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG21 | 15 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG22 | 15 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD21 | 1:57:A:THR:HG23 | 15 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG21 | 15 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG22 | 15 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD22 | 1:57:A:THR:HG23 | 15 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG21 | 15 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG22 | 15 | 0.11 |
| (1,2537) | 1:23:A:LEU:HD23 | 1:57:A:THR:HG23 | 15 | 0.11 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD21 | 2 | 0.11 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD22 | 2 | 0.11 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD23 | 2 | 0.11 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD21 | 5 | 0.11 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD22 | 5 | 0.11 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD23 | 5 | 0.11 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD21 | 12 | 0.11 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD22 | 12 | 0.11 |
| (1,2530) | 1:35:A:GLN:HE21 | 1:40:A:LEU:HD23 | 12 | 0.11 |
| (1,2484) | 1:183:A:GLN:HA | 1:183:A:GLN:HB2 | 3 | 0.11 |
| (1,2484) | 1:183:A:GLN:HA | 1:183:A:GLN:HB2 | 5 | 0.11 |
| (1,2484) | 1:183:A:GLN:HA | 1:183:A:GLN:HB2 | 6 | 0.11 |
| (1,2484) | 1:183:A:GLN:HA | 1:183:A:GLN:HB2 | 10 | 0.11 |
| (1,2484) | 1:183:A:GLN:HA | 1:183:A:GLN:HB2 | 17 | 0.11 |
| (1,2484) | 1:183:A:GLN:HA | 1:183:A:GLN:HB2 | 19 | 0.11 |
| (1,2452) | 1:149:A:VAL:HG11 | 1:150:A:PRO:HG3 | 1 | 0.11 |
| (1,2452) | 1:149:A:VAL:HG12 | 1:150:A:PRO:HG3 | 1 | 0.11 |
| (1,2452) | 1:149:A:VAL:HG13 | 1:150:A:PRO:HG3 | 1 | 0.11 |
| (1,2452) | 1:149:A:VAL:HG21 | 1:150:A:PRO:HG3 | 1 | 0.11 |
| (1,2452) | 1:149:A:VAL:HG22 | 1:150:A:PRO:HG3 | 1 | 0.11 |
| (1,2452) | 1:149:A:VAL:HG23 | 1:150:A:PRO:HG3 | 1 | 0.11 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE1 | 19 | 0.11 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE2 | 19 | 0.11 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE1 | 19 | 0.11 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE2 | 19 | 0.11 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE1 | 19 | 0.11 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE2 | 19 | 0.11 |
| (1,2392) | 1:31:A:PRO:HA | 1:34:A:TYR:HA | 5 | 0.11 |
| (1,2392) | 1:31:A:PRO:HA | 1:34:A:TYR:HA | 20 | 0.11 |
| (1,2379) | 1:55:A:LYS:H | 1:55:A:LYS:HG2 | 18 | 0.11 |
| (1,2379) | 1:55:A:LYS:H | 1:55:A:LYS:HG3 | 18 | 0.11 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 1 | 0.11 |
| (1,2328) | 1:3:A:ILE:HG21 | 1:184:A:LEU:HG | 1 | 0.11 |
| (1,2328) | 1:3:A:ILE:HG22 | 1:184:A:LEU:HG | 1 | 0.11 |
| (1,2328) | 1:3:A:ILE:HG23 | 1:184:A:LEU:HG | 1 | 0.11 |
| (1,2315) | 1:46:A:VAL:HG21 | 1:50:A:LEU:HG | 11 | 0.11 |
| (1,2315) | 1:46:A:VAL:HG22 | 1:50:A:LEU:HG | 11 | 0.11 |
| (1,2315) | 1:46:A:VAL:HG23 | 1:50:A:LEU:HG | 11 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 5 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 5 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 5 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 6 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 6 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 6 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 8 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 8 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 8 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 9 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 9 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 9 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 10 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 10 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 10 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 11 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 11 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 11 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 14 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 14 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 14 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 15 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 15 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 15 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 17 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 17 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 17 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 18 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 18 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 18 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 19 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 19 | 0.11 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 19 | 0.11 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD11 | 1 | 0.11 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD12 | 1 | 0.11 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD13 | 1 | 0.11 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD21 | 1 | 0.11 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD22 | 1 | 0.11 |
| (1,2266) | 1:78:A:ALA:H | 1:133:A:LEU:HD23 | 1 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG21 | 3 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG22 | 3 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG23 | 3 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG21 | 4 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG22 | 4 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG23 | 4 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG21 | 11 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG22 | 11 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG23 | 11 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG21 | 19 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG22 | 19 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG23 | 19 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG21 | 20 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG22 | 20 | 0.11 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG23 | 20 | 0.11 |
| (1,2226) | 1:111:A:PHE:HA | 1:116:A:VAL:HG11 | 5 | 0.11 |
| (1,2226) | 1:111:A:PHE:HA | 1:116:A:VAL:HG12 | 5 | 0.11 |
| (1,2226) | 1:111:A:PHE:HA | 1:116:A:VAL:HG13 | 5 | 0.11 |
| (1,2226) | 1:111:A:PHE:HA | 1:116:A:VAL:HG11 | 6 | 0.11 |
| (1,2226) | 1:111:A:PHE:HA | 1:116:A:VAL:HG12 | 6 | 0.11 |
| (1,2226) | 1:111:A:PHE:HA | 1:116:A:VAL:HG13 | 6 | 0.11 |
| (1,2226) | 1:111:A:PHE:HA | 1:116:A:VAL:HG11 | 20 | 0.11 |
| (1,2226) | 1:111:A:PHE:HA | 1:116:A:VAL:HG12 | 20 | 0.11 |
| (1,2226) | 1:111:A:PHE:HA | 1:116:A:VAL:HG13 | 20 | 0.11 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE1 | 8 | 0.11 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE2 | 8 | 0.11 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE3 | 8 | 0.11 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE1 | 8 | 0.11 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE2 | 8 | 0.11 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE3 | 8 | 0.11 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE1 | 11 | 0.11 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE2 | 11 | 0.11 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE3 | 11 | 0.11 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE1 | 11 | 0.11 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE2 | 11 | 0.11 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE3 | 11 | 0.11 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE1 | 20 | 0.11 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE2 | 20 | 0.11 |
| (1,2186) | 1:43:A:SER:HB2 | 1:152:A:MET:HE3 | 20 | 0.11 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE1 | 20 | 0.11 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE2 | 20 | 0.11 |
| (1,2186) | 1:43:A:SER:HB3 | 1:152:A:MET:HE3 | 20 | 0.11 |
| (1,2176) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HD2 | 1 | 0.11 |
| (1,2176) | 1:15:A:PRO:HG2 | 1:157:A:LYS:HD3 | 1 | 0.11 |
| (1,2176) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HD2 | 1 | 0.11 |
| (1,2176) | 1:15:A:PRO:HG3 | 1:157:A:LYS:HD3 | 1 | 0.11 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD11 | 4 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD12 | 4 | 0.11 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD13 | 4 | 0.11 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD11 | 17 | 0.11 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD12 | 17 | 0.11 |
| (1,2143) | 1:28:A:PHE:HB2 | 1:71:A:LEU:HD13 | 17 | 0.11 |
| (1,2126) | 1:47:A:ARG:H | 1:47:A:ARG:HG3 | 1 | 0.11 |
| (1,2115) | 1:10:A:ILE:H | 1:10:A:ILE:HG13 | 5 | 0.11 |
| (1,2072) | 1:93:A:GLU:HA | 1:97:A:LYS:HD2 | 2 | 0.11 |
| (1,2067) | 1:93:A:GLU:HA | 1:97:A:LYS:HD3 | 2 | 0.11 |
| (1,2059) | 1:49:A:LYS:H | 1:49:A:LYS:HD2 | 1 | 0.11 |
| (1,2059) | 1:49:A:LYS:H | 1:49:A:LYS:HD2 | 9 | 0.11 |
| (1,2052) | 1:55:A:LYS:H | 1:55:A:LYS:HD2 | 12 | 0.11 |
| (1,2052) | 1:55:A:LYS:H | 1:55:A:LYS:HD3 | 12 | 0.11 |
| (1,2039) | 1:27:A:SER:HB2 | 1:61:A:VAL:HA | 1 | 0.11 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 5 | 0.11 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 11 | 0.11 |
| (1,1958) | 1:107:A:ILE:HA | 1:107:A:ILE:HG13 | 14 | 0.11 |
| (1,1947) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HD2 | 4 | 0.11 |
| (1,1947) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HD3 | 4 | 0.11 |
| (1,1930) | 1:186:A:GLU:HB3 | 1:187:A:LYS:H | 8 | 0.11 |
| (1,1916) | 1:91:A:MET:HB2 | 1:92:A:PHE:HE1 | 9 | 0.11 |
| (1,1916) | 1:91:A:MET:HB2 | 1:92:A:PHE:HE2 | 9 | 0.11 |
| (1,1916) | 1:91:A:MET:HB2 | 1:92:A:PHE:HE1 | 15 | 0.11 |
| (1,1916) | 1:91:A:MET:HB2 | 1:92:A:PHE:HE2 | 15 | 0.11 |
| (1,1916) | 1:91:A:MET:HB2 | 1:92:A:PHE:HE1 | 18 | 0.11 |
| (1,1916) | 1:91:A:MET:HB2 | 1:92:A:PHE:HE2 | 18 | 0.11 |
| (1,1908) | 1:31:A:PRO:HA | 1:34:A:TYR:HB3 | 13 | 0.11 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB2 | 12 | 0.11 |
| (1,1907) | 1:46:A:VAL:HG21 | 1:47:A:ARG:HB3 | 12 | 0.11 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB2 | 12 | 0.11 |
| (1,1907) | 1:46:A:VAL:HG22 | 1:47:A:ARG:HB3 | 12 | 0.11 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB2 | 12 | 0.11 |
| (1,1907) | 1:46:A:VAL:HG23 | 1:47:A:ARG:HB3 | 12 | 0.11 |
| (1,1873) | 1:46:A:VAL:HA | 1:49:A:LYS:HB3 | 7 | 0.11 |
| (1,1837) | 1:42:A:VAL:HG11 | 1:174:A:VAL:HB | 18 | 0.11 |
| (1,1837) | 1:42:A:VAL:HG12 | 1:174:A:VAL:HB | 18 | 0.11 |
| (1,1837) | 1:42:A:VAL:HG13 | 1:174:A:VAL:HB | 18 | 0.11 |
| (1,1832) | 1:124:A:ALA:HB1 | 1:130:A:VAL:HB | 17 | 0.11 |
| (1,1832) | 1:124:A:ALA:HB2 | 1:130:A:VAL:HB | 17 | 0.11 |
| (1,1832) | 1:124:A:ALA:HB3 | 1:130:A:VAL:HB | 17 | 0.11 |
| (1,1832) | 1:124:A:ALA:HB1 | 1:130:A:VAL:HB | 20 | 0.11 |
| (1,1832) | 1:124:A:ALA:HB2 | 1:130:A:VAL:HB | 20 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1832) | 1:124:A:ALA:HB3 | 1:130:A:VAL:HB | 20 | 0.11 |
| (1,1829) | 1:169:A:ASN:HB3 | 1:172:A:VAL:HB | 8 | 0.11 |
| (1,1805) | 1:162:A:PRO:HB3 | 1:163:A:GLN:H | 17 | 0.11 |
| (1,1803) | 1:31:A:PRO:HB2 | 1:96:A:GLN:HE21 | 16 | 0.11 |
| (1,1803) | 1:31:A:PRO:HB3 | 1:96:A:GLN:HE21 | 16 | 0.11 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE1 | 5 | 0.11 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE2 | 5 | 0.11 |
| (1,1801) | 1:162:A:PRO:HB2 | 1:165:A:MET:HE3 | 5 | 0.11 |
| (1,1791) | 1:56:A:MET:HA | 1:56:A:MET:HG3 | 4 | 0.11 |
| (1,1758) | 1:14:A:LYS:H | 1:14:A:LYS:HB3 | 17 | 0.11 |
| (1,1730) | 1:55:A:LYS:H | 1:55:A:LYS:HB3 | 3 | 0.11 |
| (1,1725) | 1:24:A:GLU:HB2 | 1:58:A:LYS:HG2 | 5 | 0.11 |
| (1,1725) | 1:24:A:GLU:HB2 | 1:58:A:LYS:HG3 | 5 | 0.11 |
| (1,1725) | 1:24:A:GLU:HB3 | 1:58:A:LYS:HG2 | 5 | 0.11 |
| (1,1725) | 1:24:A:GLU:HB3 | 1:58:A:LYS:HG3 | 5 | 0.11 |
| (1,1703) | 1:59:A:TYR:HE1 | 1:136:A:GLN:HG3 | 3 | 0.11 |
| (1,1703) | 1:59:A:TYR:HE2 | 1:136:A:GLN:HG3 | 3 | 0.11 |
| (1,1695) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HE22 | 20 | 0.11 |
| (1,1685) | 1:99:A:GLN:HA | 1:99:A:GLN:HG3 | 1 | 0.11 |
| (1,1635) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HG3 | 15 | 0.11 |
| (1,1635) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HG3 | 15 | 0.11 |
| (1,1635) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HG3 | 15 | 0.11 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE1 | 11 | 0.11 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE2 | 11 | 0.11 |
| (1,1587) | 1:51:A:PRO:HA | 1:52:A:GLU:HG2 | 10 | 0.11 |
| (1,1587) | 1:51:A:PRO:HA | 1:52:A:GLU:HG3 | 10 | 0.11 |
| (1,1587) | 1:51:A:PRO:HA | 1:52:A:GLU:HG2 | 12 | 0.11 |
| (1,1587) | 1:51:A:PRO:HA | 1:52:A:GLU:HG3 | 12 | 0.11 |
| (1,1587) | 1:51:A:PRO:HA | 1:52:A:GLU:HG2 | 13 | 0.11 |
| (1,1587) | 1:51:A:PRO:HA | 1:52:A:GLU:HG3 | 13 | 0.11 |
| (1,1587) | 1:51:A:PRO:HA | 1:52:A:GLU:HG2 | 15 | 0.11 |
| (1,1587) | 1:51:A:PRO:HA | 1:52:A:GLU:HG3 | 15 | 0.11 |
| (1,1587) | 1:51:A:PRO:HA | 1:52:A:GLU:HG2 | 18 | 0.11 |
| (1,1587) | 1:51:A:PRO:HA | 1:52:A:GLU:HG3 | 18 | 0.11 |
| (1,1587) | 1:51:A:PRO:HA | 1:52:A:GLU:HG2 | 19 | 0.11 |
| (1,1587) | 1:51:A:PRO:HA | 1:52:A:GLU:HG3 | 19 | 0.11 |
| (1,1576) | 1:119:A:GLU:HG2 | 1:120:A:ASP:H | 17 | 0.11 |
| (1,1565) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 7 | 0.11 |
| (1,1545) | 1:186:A:GLU:HG3 | 1:187:A:LYS:HD3 | 12 | 0.11 |
| (1,1526) | 1:63:A:PHE:HB2 | 1:64:A:LEU:H | 7 | 0.11 |
| (1,1513) | 1:116:A:VAL:HG21 | 1:121:A:TYR:HB2 | 6 | 0.11 |
| (1,1513) | 1:116:A:VAL:HG22 | 1:121:A:TYR:HB2 | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1513) | 1:116:A:VAL:HG23 | 1:121:A:TYR:HB2 | 6 | 0.11 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG11 | 11 | 0.11 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG12 | 11 | 0.11 |
| (1,1497) | 1:111:A:PHE:HB2 | 1:112:A:VAL:HG13 | 11 | 0.11 |
| (1,1481) | 1:10:A:ILE:HG13 | 1:161:A:ASN:HB3 | 11 | 0.11 |
| (1,1470) | 1:173:A:PHE:HB3 | 1:174:A:VAL:HG11 | 8 | 0.11 |
| (1,1470) | 1:173:A:PHE:HB3 | 1:174:A:VAL:HG12 | 8 | 0.11 |
| (1,1470) | 1:173:A:PHE:HB3 | 1:174:A:VAL:HG13 | 8 | 0.11 |
| (1,1450) | 1:42:A:VAL:HA | 1:45:A:ASN:HB3 | 13 | 0.11 |
| (1,1431) | 1:85:A:ASP:HB3 | 1:87:A:ILE:H | 6 | 0.11 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB2 | 1 | 0.11 |
| (1,1395) | 1:59:A:TYR:HB2 | 1:137:A:GLN:HB3 | 1 | 0.11 |
| (1,1361) | 1:178:A:ALA:HB1 | 1:179:A:ASP:HB2 | 1 | 0.11 |
| (1,1361) | 1:178:A:ALA:HB2 | 1:179:A:ASP:HB2 | 1 | 0.11 |
| (1,1361) | 1:178:A:ALA:HB3 | 1:179:A:ASP:HB2 | 1 | 0.11 |
| (1,1361) | 1:178:A:ALA:HB1 | 1:179:A:ASP:HB2 | 18 | 0.11 |
| (1,1361) | 1:178:A:ALA:HB2 | 1:179:A:ASP:HB2 | 18 | 0.11 |
| (1,1361) | 1:178:A:ALA:HB3 | 1:179:A:ASP:HB2 | 18 | 0.11 |
| (1,1354) | 1:73:A:GLN:HE22 | 1:131:A:LYS:HE2 | 9 | 0.11 |
| (1,1354) | 1:73:A:GLN:HE22 | 1:131:A:LYS:HE3 | 9 | 0.11 |
| (1,1354) | 1:73:A:GLN:HE22 | 1:131:A:LYS:HE2 | 17 | 0.11 |
| (1,1354) | 1:73:A:GLN:HE22 | 1:131:A:LYS:HE3 | 17 | 0.11 |
| (1,1347) | 1:131:A:LYS:HG3 | 1:131:A:LYS:HE2 | 20 | 0.11 |
| (1,1347) | 1:131:A:LYS:HG3 | 1:131:A:LYS:HE3 | 20 | 0.11 |
| (1,1294) | 1:71:A:LEU:HB2 | 1:74:A:ALA:H | 14 | 0.11 |
| (1,1265) | 1:64:A:LEU:HB3 | 1:65:A:GLY:HA2 | 13 | 0.11 |
| (1,1223) | 1:161:A:ASN:HB2 | 1:164:A:GLY:H | 18 | 0.11 |
| (1,1215) | 1:73:A:GLN:HE21 | 1:77:A:VAL:HG21 | 13 | 0.11 |
| (1,1215) | 1:73:A:GLN:HE21 | 1:77:A:VAL:HG22 | 13 | 0.11 |
| (1,1215) | 1:73:A:GLN:HE21 | 1:77:A:VAL:HG23 | 13 | 0.11 |
| (1,1213) | 1:95:A:VAL:HG21 | 1:96:A:GLN:HE21 | 12 | 0.11 |
| (1,1213) | 1:95:A:VAL:HG22 | 1:96:A:GLN:HE21 | 12 | 0.11 |
| (1,1213) | 1:95:A:VAL:HG23 | 1:96:A:GLN:HE21 | 12 | 0.11 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 4 | 0.11 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 5 | 0.11 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 8 | 0.11 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 9 | 0.11 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 10 | 0.11 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 18 | 0.11 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 19 | 0.11 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 20 | 0.11 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG11 | 16 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG12 | 16 | 0.11 |
| (1,1167) | 1:27:A:SER:H | 1:61:A:VAL:HG13 | 16 | 0.11 |
| (1,1067) | 1:38:A:GLU:H | 1:38:A:GLU:HB3 | 13 | 0.11 |
| (1,1040) | 1:52:A:GLU:HB3 | 1:53:A:GLY:H | 8 | 0.11 |
| (1,1023) | 1:183:A:GLN:HG3 | 1:183:A:GLN:HE22 | 3 | 0.11 |
| (1,1007) | 1:45:A:ASN:HA | 1:48:A:GLN:H | 7 | 0.11 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 4 | 0.11 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 11 | 0.11 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 12 | 0.11 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 14 | 0.11 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 16 | 0.11 |
| (1,985) | 1:93:A:GLU:HB2 | 1:95:A:VAL:H | 9 | 0.11 |
| (1,985) | 1:93:A:GLU:HB3 | 1:95:A:VAL:H | 9 | 0.11 |
| (1,970) | 1:123:A:ALA:HB1 | 1:126:A:ASN:HD21 | 4 | 0.11 |
| (1,970) | 1:123:A:ALA:HB2 | 1:126:A:ASN:HD21 | 4 | 0.11 |
| (1,970) | 1:123:A:ALA:HB3 | 1:126:A:ASN:HD21 | 4 | 0.11 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 19 | 0.11 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 19 | 0.11 |
| (1,941) | 1:35:A:GLN:HG2 | 1:40:A:LEU:H | 20 | 0.11 |
| (1,941) | 1:35:A:GLN:HG3 | 1:40:A:LEU:H | 20 | 0.11 |
| (1,936) | 1:117:A:LYS:HG3 | 1:118:A:GLY:H | 1 | 0.11 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD21 | 2 | 0.11 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD22 | 2 | 0.11 |
| (1,924) | 1:183:A:GLN:H | 1:184:A:LEU:HD23 | 2 | 0.11 |
| (1,892) | 1:101:A:VAL:HA | 1:103:A:SER:H | 3 | 0.11 |
| (1,869) | 1:145:A:GLN:H | 1:146:A:LEU:HB2 | 19 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 1 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 2 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 3 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 4 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 5 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 6 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 8 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 9 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 10 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 11 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 12 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 13 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 15 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 16 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 17 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 18 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 19 | 0.11 |
| (1,841) | 1:184:A:LEU:HB3 | 1:186:A:GLU:H | 20 | 0.11 |
| (1,809) | 1:179:A:ASP:HA | 1:180:A:THR:H | 2 | 0.11 |
| (1,809) | 1:179:A:ASP:HA | 1:180:A:THR:H | 4 | 0.11 |
| (1,809) | 1:179:A:ASP:HA | 1:180:A:THR:H | 6 | 0.11 |
| (1,809) | 1:179:A:ASP:HA | 1:180:A:THR:H | 9 | 0.11 |
| (1,795) | 1:176:A:GLN:HA | 1:179:A:ASP:H | 13 | 0.11 |
| (1,795) | 1:176:A:GLN:HA | 1:179:A:ASP:H | 16 | 0.11 |
| (1,791) | 1:169:A:ASN:H | 1:170:A:MET:HE1 | 1 | 0.11 |
| (1,791) | 1:169:A:ASN:H | 1:170:A:MET:HE2 | 1 | 0.11 |
| (1,791) | 1:169:A:ASN:H | 1:170:A:MET:HE3 | 1 | 0.11 |
| (1,778) | 1:51:A:PRO:HB3 | 1:54:A:THR:H | 8 | 0.11 |
| (1,778) | 1:51:A:PRO:HB3 | 1:54:A:THR:H | 10 | 0.11 |
| (1,778) | 1:51:A:PRO:HB3 | 1:54:A:THR:H | 13 | 0.11 |
| (1,778) | 1:51:A:PRO:HB3 | 1:54:A:THR:H | 16 | 0.11 |
| (1,778) | 1:51:A:PRO:HB3 | 1:54:A:THR:H | 19 | 0.11 |
| (1,737) | 1:31:A:PRO:HA | 1:35:A:GLN:H | 14 | 0.11 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 5 | 0.11 |
| (1,682) | 1:69:A:LYS:HA | 1:71:A:LEU:H | 20 | 0.11 |
| (1,642) | 1:75:A:TRP:HB2 | 1:76:A:ALA:H | 4 | 0.11 |
| (1,599) | 1:183:A:GLN:HB3 | 1:184:A:LEU:H | 15 | 0.11 |
| (1,588) | 1:175:A:ALA:HB1 | 1:178:A:ALA:H | 10 | 0.11 |
| (1,588) | 1:175:A:ALA:HB2 | 1:178:A:ALA:H | 10 | 0.11 |
| (1,588) | 1:175:A:ALA:HB3 | 1:178:A:ALA:H | 10 | 0.11 |
| (1,584) | 1:47:A:ARG:H | 1:47:A:ARG:HD3 | 1 | 0.11 |
| (1,577) | 1:121:A:TYR:HB2 | 1:122:A:ASP:H | 10 | 0.11 |
| (1,573) | 1:49:A:LYS:HG2 | 1:50:A:LEU:H | 15 | 0.11 |
| (1,573) | 1:49:A:LYS:HG3 | 1:50:A:LEU:H | 15 | 0.11 |
| (1,565) | 1:163:A:GLN:HA | 1:165:A:MET:H | 1 | 0.11 |
| (1,560) | 1:42:A:VAL:HG21 | 1:178:A:ALA:H | 12 | 0.11 |
| (1,560) | 1:42:A:VAL:HG22 | 1:178:A:ALA:H | 12 | 0.11 |
| (1,560) | 1:42:A:VAL:HG23 | 1:178:A:ALA:H | 12 | 0.11 |
| (1,516) | 1:26:A:PHE:H | 1:58:A:LYS:HG2 | 1 | 0.11 |
| (1,516) | 1:26:A:PHE:H | 1:58:A:LYS:HG3 | 1 | 0.11 |
| (1,458) | 1:88:A:THR:HA | 1:92:A:PHE:H | 9 | 0.11 |
| (1,456) | 1:60:A:HIS:HB3 | 1:75:A:TRP:H | 5 | 0.11 |
| (1,456) | 1:60:A:HIS:HB3 | 1:75:A:TRP:H | 8 | 0.11 |
| (1,456) | 1:60:A:HIS:HB3 | 1:75:A:TRP:H | 11 | 0.11 |
| (1,456) | 1:60:A:HIS:HB3 | 1:75:A:TRP:H | 13 | 0.11 |
| (1,456) | 1:60:A:HIS:HB3 | 1:75:A:TRP:H | 18 | 0.11 |
| (1,456) | 1:60:A:HIS:HB3 | 1:75:A:TRP:H | 19 | 0.11 |
| (1,456) | 1:60:A:HIS:HB3 | 1:75:A:TRP:H | 20 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,445) | 1:169:A:ASN:HD21 | 1:171:A:ASP:H | 2 | 0.11 |
| (1,445) | 1:169:A:ASN:HD21 | 1:171:A:ASP:H | 3 | 0.11 |
| (1,445) | 1:169:A:ASN:HD21 | 1:171:A:ASP:H | 4 | 0.11 |
| (1,445) | 1:169:A:ASN:HD21 | 1:171:A:ASP:H | 6 | 0.11 |
| (1,445) | 1:169:A:ASN:HD21 | 1:171:A:ASP:H | 8 | 0.11 |
| (1,445) | 1:169:A:ASN:HD21 | 1:171:A:ASP:H | 11 | 0.11 |
| (1,445) | 1:169:A:ASN:HD21 | 1:171:A:ASP:H | 12 | 0.11 |
| (1,445) | 1:169:A:ASN:HD21 | 1:171:A:ASP:H | 14 | 0.11 |
| (1,445) | 1:169:A:ASN:HD21 | 1:171:A:ASP:H | 16 | 0.11 |
| (1,441) | 1:34:A:TYR:HE2 | 1:92:A:PHE:H | 2 | 0.11 |
| (1,413) | 1:77:A:VAL:HG11 | 1:123:A:ALA:H | 9 | 0.11 |
| (1,413) | 1:77:A:VAL:HG12 | 1:123:A:ALA:H | 9 | 0.11 |
| (1,413) | 1:77:A:VAL:HG13 | 1:123:A:ALA:H | 9 | 0.11 |
| (1,408) | 1:2:A:GLN:H | 1:3:A:ILE:H | 5 | 0.11 |
| (1,408) | 1:2:A:GLN:H | 1:3:A:ILE:H | 9 | 0.11 |
| (1,408) | 1:2:A:GLN:H | 1:3:A:ILE:H | 10 | 0.11 |
| (1,408) | 1:2:A:GLN:H | 1:3:A:ILE:H | 11 | 0.11 |
| (1,408) | 1:2:A:GLN:H | 1:3:A:ILE:H | 15 | 0.11 |
| (1,408) | 1:2:A:GLN:H | 1:3:A:ILE:H | 16 | 0.11 |
| (1,408) | 1:2:A:GLN:H | 1:3:A:ILE:H | 18 | 0.11 |
| (1,335) | 1:165:A:MET:HE1 | 1:166:A:ASP:H | 16 | 0.11 |
| (1,335) | 1:165:A:MET:HE2 | 1:166:A:ASP:H | 16 | 0.11 |
| (1,335) | 1:165:A:MET:HE3 | 1:166:A:ASP:H | 16 | 0.11 |
| (1,334) | 1:165:A:MET:HG2 | 1:166:A:ASP:H | 3 | 0.11 |
| (1,334) | 1:165:A:MET:HG3 | 1:166:A:ASP:H | 3 | 0.11 |
| (1,334) | 1:165:A:MET:HG2 | 1:166:A:ASP:H | 6 | 0.11 |
| (1,334) | 1:165:A:MET:HG3 | 1:166:A:ASP:H | 6 | 0.11 |
| (1,334) | 1:165:A:MET:HG2 | 1:166:A:ASP:H | 8 | 0.11 |
| (1,334) | 1:165:A:MET:HG3 | 1:166:A:ASP:H | 8 | 0.11 |
| (1,334) | 1:165:A:MET:HG2 | 1:166:A:ASP:H | 10 | 0.11 |
| (1,334) | 1:165:A:MET:HG3 | 1:166:A:ASP:H | 10 | 0.11 |
| (1,334) | 1:165:A:MET:HG2 | 1:166:A:ASP:H | 14 | 0.11 |
| (1,334) | 1:165:A:MET:HG3 | 1:166:A:ASP:H | 14 | 0.11 |
| (1,334) | 1:165:A:MET:HG2 | 1:166:A:ASP:H | 19 | 0.11 |
| (1,334) | 1:165:A:MET:HG3 | 1:166:A:ASP:H | 19 | 0.11 |
| (1,300) | 1:130:A:VAL:HG21 | 1:131:A:LYS:H | 1 | 0.11 |
| (1,300) | 1:130:A:VAL:HG22 | 1:131:A:LYS:H | 1 | 0.11 |
| (1,300) | 1:130:A:VAL:HG23 | 1:131:A:LYS:H | 1 | 0.11 |
| (1,300) | 1:130:A:VAL:HG21 | 1:131:A:LYS:H | 14 | 0.11 |
| (1,300) | 1:130:A:VAL:HG22 | 1:131:A:LYS:H | 14 | 0.11 |
| (1,300) | 1:130:A:VAL:HG23 | 1:131:A:LYS:H | 14 | 0.11 |
| (1,287) | 1:139:A:LYS:H | 1:139:A:LYS:HG2 | 1 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,287) | 1:139:A:LYS:H | 1:139:A:LYS:HG3 | 1 | 0.11 |
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 15 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 3 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 3 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 5 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 5 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 6 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 6 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 8 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 8 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 9 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 9 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 12 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 12 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 14 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 14 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 17 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 17 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 20 | 0.11 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 20 | 0.11 |
| (1,259) | 1:69:A:LYS:HD2 | 1:70:A:ASP:H | 7 | 0.11 |
| (1,238) | 1:74:A:ALA:H | 1:107:A:ILE:HG21 | 11 | 0.11 |
| (1,238) | 1:74:A:ALA:H | 1:107:A:ILE:HG22 | 11 | 0.11 |
| (1,238) | 1:74:A:ALA:H | 1:107:A:ILE:HG23 | 11 | 0.11 |
| (1,238) | 1:74:A:ALA:H | 1:107:A:ILE:HG21 | 16 | 0.11 |
| (1,238) | 1:74:A:ALA:H | 1:107:A:ILE:HG22 | 16 | 0.11 |
| (1,238) | 1:74:A:ALA:H | 1:107:A:ILE:HG23 | 16 | 0.11 |
| (1,238) | 1:74:A:ALA:H | 1:107:A:ILE:HG21 | 17 | 0.11 |
| (1,238) | 1:74:A:ALA:H | 1:107:A:ILE:HG22 | 17 | 0.11 |
| (1,238) | 1:74:A:ALA:H | 1:107:A:ILE:HG23 | 17 | 0.11 |
| (1,235) | 1:87:A:ILE:HG21 | 1:89:A:ALA:H | 3 | 0.11 |
| (1,235) | 1:87:A:ILE:HG22 | 1:89:A:ALA:H | 3 | 0.11 |
| (1,235) | 1:87:A:ILE:HG23 | 1:89:A:ALA:H | 3 | 0.11 |
| (1,235) | 1:87:A:ILE:HG21 | 1:89:A:ALA:H | 5 | 0.11 |
| (1,235) | 1:87:A:ILE:HG22 | 1:89:A:ALA:H | 5 | 0.11 |
| (1,235) | 1:87:A:ILE:HG23 | 1:89:A:ALA:H | 5 | 0.11 |
| (1,235) | 1:87:A:ILE:HG21 | 1:89:A:ALA:H | 6 | 0.11 |
| (1,235) | 1:87:A:ILE:HG22 | 1:89:A:ALA:H | 6 | 0.11 |
| (1,235) | 1:87:A:ILE:HG23 | 1:89:A:ALA:H | 6 | 0.11 |
| (1,235) | 1:87:A:ILE:HG21 | 1:89:A:ALA:H | 9 | 0.11 |
| (1,235) | 1:87:A:ILE:HG22 | 1:89:A:ALA:H | 9 | 0.11 |
| (1,235) | 1:87:A:ILE:HG23 | 1:89:A:ALA:H | 9 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,235) | 1:87:A:ILE:HG21 | 1:89:A:ALA:H | 10 | 0.11 |
| (1,235) | 1:87:A:ILE:HG22 | 1:89:A:ALA:H | 10 | 0.11 |
| (1,235) | 1:87:A:ILE:HG23 | 1:89:A:ALA:H | 10 | 0.11 |
| (1,235) | 1:87:A:ILE:HG21 | 1:89:A:ALA:H | 11 | 0.11 |
| (1,235) | 1:87:A:ILE:HG22 | 1:89:A:ALA:H | 11 | 0.11 |
| (1,235) | 1:87:A:ILE:HG23 | 1:89:A:ALA:H | 11 | 0.11 |
| (1,235) | 1:87:A:ILE:HG21 | 1:89:A:ALA:H | 13 | 0.11 |
| (1,235) | 1:87:A:ILE:HG22 | 1:89:A:ALA:H | 13 | 0.11 |
| (1,235) | 1:87:A:ILE:HG23 | 1:89:A:ALA:H | 13 | 0.11 |
| (1,235) | 1:87:A:ILE:HG21 | 1:89:A:ALA:H | 15 | 0.11 |
| (1,235) | 1:87:A:ILE:HG22 | 1:89:A:ALA:H | 15 | 0.11 |
| (1,235) | 1:87:A:ILE:HG23 | 1:89:A:ALA:H | 15 | 0.11 |
| (1,235) | 1:87:A:ILE:HG21 | 1:89:A:ALA:H | 16 | 0.11 |
| (1,235) | 1:87:A:ILE:HG22 | 1:89:A:ALA:H | 16 | 0.11 |
| (1,235) | 1:87:A:ILE:HG23 | 1:89:A:ALA:H | 16 | 0.11 |
| (1,235) | 1:87:A:ILE:HG21 | 1:89:A:ALA:H | 19 | 0.11 |
| (1,235) | 1:87:A:ILE:HG22 | 1:89:A:ALA:H | 19 | 0.11 |
| (1,235) | 1:87:A:ILE:HG23 | 1:89:A:ALA:H | 19 | 0.11 |
| (1,235) | 1:87:A:ILE:HG21 | 1:89:A:ALA:H | 20 | 0.11 |
| (1,235) | 1:87:A:ILE:HG22 | 1:89:A:ALA:H | 20 | 0.11 |
| (1,235) | 1:87:A:ILE:HG23 | 1:89:A:ALA:H | 20 | 0.11 |
| (1,223) | 1:40:A:LEU:HD11 | 1:170:A:MET:H | 1 | 0.11 |
| (1,223) | 1:40:A:LEU:HD12 | 1:170:A:MET:H | 1 | 0.11 |
| (1,223) | 1:40:A:LEU:HD13 | 1:170:A:MET:H | 1 | 0.11 |
| (1,223) | 1:40:A:LEU:HD11 | 1:170:A:MET:H | 3 | 0.11 |
| (1,223) | 1:40:A:LEU:HD12 | 1:170:A:MET:H | 3 | 0.11 |
| (1,223) | 1:40:A:LEU:HD13 | 1:170:A:MET:H | 3 | 0.11 |
| (1,216) | 1:34:A:TYR:H | 1:96:A:GLN:HE21 | 9 | 0.11 |
| (1,211) | 1:26:A:PHE:H | 1:151:A:ALA:H | 3 | 0.11 |
| (1,211) | 1:26:A:PHE:H | 1:151:A:ALA:H | 13 | 0.11 |
| (1,185) | 1:59:A:TYR:HB2 | 1:60:A:HIS:H | 6 | 0.11 |
| (1,175) | 1:87:A:ILE:HG21 | 1:113:A:ASP:H | 2 | 0.11 |
| (1,175) | 1:87:A:ILE:HG22 | 1:113:A:ASP:H | 2 | 0.11 |
| (1,175) | 1:87:A:ILE:HG23 | 1:113:A:ASP:H | 2 | 0.11 |
| (1,175) | 1:87:A:ILE:HG21 | 1:113:A:ASP:H | 10 | 0.11 |
| (1,175) | 1:87:A:ILE:HG22 | 1:113:A:ASP:H | 10 | 0.11 |
| (1,175) | 1:87:A:ILE:HG23 | 1:113:A:ASP:H | 10 | 0.11 |
| (1,175) | 1:87:A:ILE:HG21 | 1:113:A:ASP:H | 11 | 0.11 |
| (1,175) | 1:87:A:ILE:HG22 | 1:113:A:ASP:H | 11 | 0.11 |
| (1,175) | 1:87:A:ILE:HG23 | 1:113:A:ASP:H | 11 | 0.11 |
| (1,175) | 1:87:A:ILE:HG21 | 1:113:A:ASP:H | 14 | 0.11 |
| (1,175) | 1:87:A:ILE:HG22 | 1:113:A:ASP:H | 14 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,175) | 1:87:A:ILE:HG23 | 1:113:A:ASP:H | 14 | 0.11 |
| (1,175) | 1:87:A:ILE:HG21 | 1:113:A:ASP:H | 17 | 0.11 |
| (1,175) | 1:87:A:ILE:HG22 | 1:113:A:ASP:H | 17 | 0.11 |
| (1,175) | 1:87:A:ILE:HG23 | 1:113:A:ASP:H | 17 | 0.11 |
| (1,175) | 1:87:A:ILE:HG21 | 1:113:A:ASP:H | 19 | 0.11 |
| (1,175) | 1:87:A:ILE:HG22 | 1:113:A:ASP:H | 19 | 0.11 |
| (1,175) | 1:87:A:ILE:HG23 | 1:113:A:ASP:H | 19 | 0.11 |
| (1,174) | 1:110:A:VAL:HG21 | 1:113:A:ASP:H | 10 | 0.11 |
| (1,174) | 1:110:A:VAL:HG22 | 1:113:A:ASP:H | 10 | 0.11 |
| (1,174) | 1:110:A:VAL:HG23 | 1:113:A:ASP:H | 10 | 0.11 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD21 | 20 | 0.11 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD22 | 20 | 0.11 |
| (1,151) | 1:133:A:LEU:H | 1:133:A:LEU:HD23 | 20 | 0.11 |
| (1,138) | 1:80:A:ALA:H | 1:81:A:LEU:HA | 10 | 0.11 |
| (1,138) | 1:80:A:ALA:H | 1:81:A:LEU:HA | 18 | 0.11 |
| (1,126) | 1:10:A:ILE:HG21 | 1:159:A:GLN:H | 1 | 0.11 |
| (1,126) | 1:10:A:ILE:HG22 | 1:159:A:GLN:H | 1 | 0.11 |
| (1,126) | 1:10:A:ILE:HG23 | 1:159:A:GLN:H | 1 | 0.11 |
| (1,126) | 1:10:A:ILE:HG21 | 1:159:A:GLN:H | 17 | 0.11 |
| (1,126) | 1:10:A:ILE:HG22 | 1:159:A:GLN:H | 17 | 0.11 |
| (1,126) | 1:10:A:ILE:HG23 | 1:159:A:GLN:H | 17 | 0.11 |
| (1,107) | 1:0:A:ASN:HA | 1:1:A:ALA:H | 20 | 0.11 |
| (1,92) | 1:188:A:LYS:H | 1:188:A:LYS:HB2 | 9 | 0.11 |
| (1,92) | 1:188:A:LYS:H | 1:188:A:LYS:HB3 | 9 | 0.11 |
| (1,91) | 1:187:A:LYS:H | 1:188:A:LYS:H | 15 | 0.11 |
| (1,91) | 1:187:A:LYS:H | 1:188:A:LYS:H | 18 | 0.11 |
| (1,62) | 1:102:A:GLN:H | 1:102:A:GLN:HG2 | 3 | 0.11 |
| (1,28) | 1:58:A:LYS:HG2 | 1:75:A:TRP:HE1 | 16 | 0.11 |
| (1,28) | 1:58:A:LYS:HG3 | 1:75:A:TRP:HE1 | 16 | 0.11 |
| (1,25) | 1:59:A:TYR:HE1 | 1:75:A:TRP:HE1 | 15 | 0.11 |
| (1,25) | 1:59:A:TYR:HE2 | 1:75:A:TRP:HE1 | 15 | 0.11 |
| (1,3531) | 1:58:A:LYS:H | 1:75:A:TRP:HZ2 | 5 | 0.1 |
| (1,3521) | 1:162:A:PRO:HG2 | 1:177:A:TYR:HE1 | 20 | 0.1 |
| (1,3521) | 1:162:A:PRO:HG2 | 1:177:A:TYR:HE2 | 20 | 0.1 |
| (1,3521) | 1:162:A:PRO:HG3 | 1:177:A:TYR:HE1 | 20 | 0.1 |
| (1,3521) | 1:162:A:PRO:HG3 | 1:177:A:TYR:HE2 | 20 | 0.1 |
| (1,3494) | 1:59:A:TYR:HE1 | 1:137:A:GLN:HG3 | 13 | 0.1 |
| (1,3494) | 1:59:A:TYR:HE2 | 1:137:A:GLN:HG3 | 13 | 0.1 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE1 | 9 | 0.1 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE2 | 9 | 0.1 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE1 | 15 | 0.1 |
| (1,3483) | 1:29:A:TYR:HA | 1:29:A:TYR:HE2 | 15 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3461) | 1:75:A:TRP:HB3 | 1:75:A:TRP:HE3 | 9 | 0.1 |
| (1,3419) | 1:75:A:TRP:HB2 | 1:75:A:TRP:HD1 | 11 | 0.1 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD11 | 14 | 0.1 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD12 | 14 | 0.1 |
| (1,3416) | 1:59:A:TYR:HD1 | 1:79:A:ILE:HD13 | 14 | 0.1 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD11 | 14 | 0.1 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD12 | 14 | 0.1 |
| (1,3416) | 1:59:A:TYR:HD2 | 1:79:A:ILE:HD13 | 14 | 0.1 |
| (1,3414) | 1:59:A:TYR:HD1 | 1:137:A:GLN:HB2 | 11 | 0.1 |
| (1,3414) | 1:59:A:TYR:HD1 | 1:137:A:GLN:HB3 | 11 | 0.1 |
| (1,3414) | 1:59:A:TYR:HD2 | 1:137:A:GLN:HB2 | 11 | 0.1 |
| (1,3414) | 1:59:A:TYR:HD2 | 1:137:A:GLN:HB3 | 11 | 0.1 |
| (1,3404) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HB2 | 14 | 0.1 |
| (1,3404) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HB3 | 14 | 0.1 |
| (1,3404) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HB2 | 14 | 0.1 |
| (1,3404) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HB3 | 14 | 0.1 |
| (1,3398) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HG2 | 20 | 0.1 |
| (1,3398) | 1:26:A:PHE:HD1 | 1:58:A:LYS:HG3 | 20 | 0.1 |
| (1,3398) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HG2 | 20 | 0.1 |
| (1,3398) | 1:26:A:PHE:HD2 | 1:58:A:LYS:HG3 | 20 | 0.1 |
| (1,3388) | 1:34:A:TYR:HD1 | 1:92:A:PHE:HA | 10 | 0.1 |
| (1,3388) | 1:34:A:TYR:HD2 | 1:92:A:PHE:HA | 10 | 0.1 |
| (1,3365) | 1:177:A:TYR:HD1 | 1:181:A:VAL:H | 1 | 0.1 |
| (1,3365) | 1:177:A:TYR:HD2 | 1:181:A:VAL:H | 1 | 0.1 |
| (1,3286) | 1:81:A:LEU:HB2 | 1:82:A:GLY:HA3 | 9 | 0.1 |
| (1,3230) | 1:87:A:ILE:HA | 1:90:A:PRO:HD3 | 7 | 0.1 |
| (1,3221) | 1:87:A:ILE:HD11 | 1:88:A:THR:HA | 1 | 0.1 |
| (1,3221) | 1:87:A:ILE:HD12 | 1:88:A:THR:HA | 1 | 0.1 |
| (1,3221) | 1:87:A:ILE:HD13 | 1:88:A:THR:HA | 1 | 0.1 |
| (1,3221) | 1:87:A:ILE:HD11 | 1:88:A:THR:HA | 17 | 0.1 |
| (1,3221) | 1:87:A:ILE:HD12 | 1:88:A:THR:HA | 17 | 0.1 |
| (1,3221) | 1:87:A:ILE:HD13 | 1:88:A:THR:HA | 17 | 0.1 |
| (1,3220) | 1:87:A:ILE:HA | 1:87:A:ILE:HD11 | 15 | 0.1 |
| (1,3220) | 1:87:A:ILE:HA | 1:87:A:ILE:HD12 | 15 | 0.1 |
| (1,3220) | 1:87:A:ILE:HA | 1:87:A:ILE:HD13 | 15 | 0.1 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD11 | 4 | 0.1 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD12 | 4 | 0.1 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD13 | 4 | 0.1 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD11 | 8 | 0.1 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD12 | 8 | 0.1 |
| (1,3178) | 1:71:A:LEU:HA | 1:107:A:ILE:HD13 | 8 | 0.1 |
| (1,3175) | 1:104:A:VAL:H | 1:107:A:ILE:HD11 | 6 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3175) | 1:104:A:VAL:H | 1:107:A:ILE:HD12 | 6 | 0.1 |
| (1,3175) | 1:104:A:VAL:H | 1:107:A:ILE:HD13 | 6 | 0.1 |
| (1,3169) | 1:88:A:THR:H | 1:89:A:ALA:HB1 | 6 | 0.1 |
| (1,3169) | 1:88:A:THR:H | 1:89:A:ALA:HB2 | 6 | 0.1 |
| (1,3169) | 1:88:A:THR:H | 1:89:A:ALA:HB3 | 6 | 0.1 |
| (1,3169) | 1:88:A:THR:H | 1:89:A:ALA:HB1 | 12 | 0.1 |
| (1,3169) | 1:88:A:THR:H | 1:89:A:ALA:HB2 | 12 | 0.1 |
| (1,3169) | 1:88:A:THR:H | 1:89:A:ALA:HB3 | 12 | 0.1 |
| (1,3116) | 1:23:A:LEU:HA | 1:57:A:THR:H | 14 | 0.1 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB1 | 5 | 0.1 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB2 | 5 | 0.1 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB3 | 5 | 0.1 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB1 | 11 | 0.1 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB2 | 11 | 0.1 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB3 | 11 | 0.1 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB1 | 17 | 0.1 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB2 | 17 | 0.1 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB3 | 17 | 0.1 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB1 | 18 | 0.1 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB2 | 18 | 0.1 |
| (1,3099) | 1:134:A:VAL:HB | 1:135:A:ALA:HB3 | 18 | 0.1 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB1 | 9 | 0.1 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB2 | 9 | 0.1 |
| (1,3063) | 1:46:A:VAL:HG11 | 1:178:A:ALA:HB3 | 9 | 0.1 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB1 | 9 | 0.1 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB2 | 9 | 0.1 |
| (1,3063) | 1:46:A:VAL:HG12 | 1:178:A:ALA:HB3 | 9 | 0.1 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB1 | 9 | 0.1 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB2 | 9 | 0.1 |
| (1,3063) | 1:46:A:VAL:HG13 | 1:178:A:ALA:HB3 | 9 | 0.1 |
| (1,3045) | 1:167:A:THR:HB | 1:170:A:MET:HE1 | 6 | 0.1 |
| (1,3045) | 1:167:A:THR:HB | 1:170:A:MET:HE2 | 6 | 0.1 |
| (1,3045) | 1:167:A:THR:HB | 1:170:A:MET:HE3 | 6 | 0.1 |
| (1,3033) | 1:107:A:ILE:HG21 | 1:108:A:ARG:HA | 9 | 0.1 |
| (1,3033) | 1:107:A:ILE:HG22 | 1:108:A:ARG:HA | 9 | 0.1 |
| (1,3033) | 1:107:A:ILE:HG23 | 1:108:A:ARG:HA | 9 | 0.1 |
| (1,3018) | 1:170:A:MET:HB3 | 1:170:A:MET:HE1 | 2 | 0.1 |
| (1,3018) | 1:170:A:MET:HB3 | 1:170:A:MET:HE2 | 2 | 0.1 |
| (1,3018) | 1:170:A:MET:HB3 | 1:170:A:MET:HE3 | 2 | 0.1 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD21 | 2 | 0.1 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD22 | 2 | 0.1 |
| (1,3005) | 1:160:A:LEU:HA | 1:184:A:LEU:HD23 | 2 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB1 | 16 | 0.1 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB2 | 16 | 0.1 |
| (1,3002) | 1:139:A:LYS:HG2 | 1:140:A:ALA:HB3 | 16 | 0.1 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB1 | 16 | 0.1 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB2 | 16 | 0.1 |
| (1,3002) | 1:139:A:LYS:HG3 | 1:140:A:ALA:HB3 | 16 | 0.1 |
| (1,2996) | 1:140:A:ALA:HB1 | 1:141:A:ALA:H | 11 | 0.1 |
| (1,2996) | 1:140:A:ALA:HB2 | 1:141:A:ALA:H | 11 | 0.1 |
| (1,2996) | 1:140:A:ALA:HB3 | 1:141:A:ALA:H | 11 | 0.1 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB1 | 5 | 0.1 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB2 | 5 | 0.1 |
| (1,2984) | 1:86:A:LYS:HB2 | 1:114:A:ALA:HB3 | 5 | 0.1 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB1 | 5 | 0.1 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB2 | 5 | 0.1 |
| (1,2984) | 1:86:A:LYS:HB3 | 1:114:A:ALA:HB3 | 5 | 0.1 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD11 | 20 | 0.1 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD12 | 20 | 0.1 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD13 | 20 | 0.1 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD21 | 20 | 0.1 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD22 | 20 | 0.1 |
| (1,2969) | 1:144:A:LEU:HA | 1:144:A:LEU:HD23 | 20 | 0.1 |
| (1,2959) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HE1 | 2 | 0.1 |
| (1,2959) | 1:3:A:ILE:HG21 | 1:9:A:TYR:HE2 | 2 | 0.1 |
| (1,2959) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HE1 | 2 | 0.1 |
| (1,2959) | 1:3:A:ILE:HG22 | 1:9:A:TYR:HE2 | 2 | 0.1 |
| (1,2959) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HE1 | 2 | 0.1 |
| (1,2959) | 1:3:A:ILE:HG23 | 1:9:A:TYR:HE2 | 2 | 0.1 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG11 | 3 | 0.1 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG12 | 3 | 0.1 |
| (1,2922) | 1:94:A:ALA:HB1 | 1:110:A:VAL:HG13 | 3 | 0.1 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG11 | 3 | 0.1 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG12 | 3 | 0.1 |
| (1,2922) | 1:94:A:ALA:HB2 | 1:110:A:VAL:HG13 | 3 | 0.1 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG11 | 3 | 0.1 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG12 | 3 | 0.1 |
| (1,2922) | 1:94:A:ALA:HB3 | 1:110:A:VAL:HG13 | 3 | 0.1 |
| (1,2879) | 1:59:A:TYR:HE1 | 1:140:A:ALA:HA | 6 | 0.1 |
| (1,2879) | 1:59:A:TYR:HE2 | 1:140:A:ALA:HA | 6 | 0.1 |
| (1,2879) | 1:59:A:TYR:HE1 | 1:140:A:ALA:HA | 8 | 0.1 |
| (1,2879) | 1:59:A:TYR:HE2 | 1:140:A:ALA:HA | 8 | 0.1 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE1 | 19 | 0.1 |
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE2 | 19 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2871) | 1:162:A:PRO:HA | 1:165:A:MET:HE3 | 19 | 0.1 |
| (1,2847) | 1:2:A:GLN:HA | 1:2:A:GLN:HB3 | 17 | 0.1 |
| (1,2803) | 1:73:A:GLN:HA | 1:76:A:ALA:HB1 | 13 | 0.1 |
| (1,2803) | 1:73:A:GLN:HA | 1:76:A:ALA:HB2 | 13 | 0.1 |
| (1,2803) | 1:73:A:GLN:HA | 1:76:A:ALA:HB3 | 13 | 0.1 |
| (1,2803) | 1:73:A:GLN:HA | 1:76:A:ALA:HB1 | 15 | 0.1 |
| (1,2803) | 1:73:A:GLN:HA | 1:76:A:ALA:HB2 | 15 | 0.1 |
| (1,2803) | 1:73:A:GLN:HA | 1:76:A:ALA:HB3 | 15 | 0.1 |
| (1,2753) | 1:61:A:VAL:HG11 | 1:62:A:GLU:HA | 2 | 0.1 |
| (1,2753) | 1:61:A:VAL:HG12 | 1:62:A:GLU:HA | 2 | 0.1 |
| (1,2753) | 1:61:A:VAL:HG13 | 1:62:A:GLU:HA | 2 | 0.1 |
| (1,2753) | 1:61:A:VAL:HG11 | 1:62:A:GLU:HA | 12 | 0.1 |
| (1,2753) | 1:61:A:VAL:HG12 | 1:62:A:GLU:HA | 12 | 0.1 |
| (1,2753) | 1:61:A:VAL:HG13 | 1:62:A:GLU:HA | 12 | 0.1 |
| (1,2742) | 1:77:A:VAL:HA | 1:130:A:VAL:HG11 | 6 | 0.1 |
| (1,2742) | 1:77:A:VAL:HA | 1:130:A:VAL:HG12 | 6 | 0.1 |
| (1,2742) | 1:77:A:VAL:HA | 1:130:A:VAL:HG13 | 6 | 0.1 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG11 | 2 | 0.1 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG12 | 2 | 0.1 |
| (1,2735) | 1:125:A:TRP:H | 1:130:A:VAL:HG13 | 2 | 0.1 |
| (1,2713) | 1:104:A:VAL:HG11 | 1:105:A:ALA:H | 10 | 0.1 |
| (1,2713) | 1:104:A:VAL:HG12 | 1:105:A:ALA:H | 10 | 0.1 |
| (1,2713) | 1:104:A:VAL:HG13 | 1:105:A:ALA:H | 10 | 0.1 |
| (1,2682) | 1:117:A:LYS:HA | 1:117:A:LYS:HB2 | 11 | 0.1 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG21 | 4 | 0.1 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG22 | 4 | 0.1 |
| (1,2654) | 1:87:A:ILE:HD11 | 1:88:A:THR:HG23 | 4 | 0.1 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG21 | 4 | 0.1 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG22 | 4 | 0.1 |
| (1,2654) | 1:87:A:ILE:HD12 | 1:88:A:THR:HG23 | 4 | 0.1 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG21 | 4 | 0.1 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG22 | 4 | 0.1 |
| (1,2654) | 1:87:A:ILE:HD13 | 1:88:A:THR:HG23 | 4 | 0.1 |
| (1,2653) | 1:38:A:GLU:HG2 | 1:88:A:THR:HG21 | 6 | 0.1 |
| (1,2653) | 1:38:A:GLU:HG2 | 1:88:A:THR:HG22 | 6 | 0.1 |
| (1,2653) | 1:38:A:GLU:HG2 | 1:88:A:THR:HG23 | 6 | 0.1 |
| (1,2621) | 1:101:A:VAL:HG21 | 1:106:A:ASP:H | 19 | 0.1 |
| (1,2621) | 1:101:A:VAL:HG22 | 1:106:A:ASP:H | 19 | 0.1 |
| (1,2621) | 1:101:A:VAL:HG23 | 1:106:A:ASP:H | 19 | 0.1 |
| (1,2607) | 1:47:A:ARG:HD2 | 1:48:A:GLN:HA | 14 | 0.1 |
| (1,2607) | 1:47:A:ARG:HD3 | 1:48:A:GLN:HA | 14 | 0.1 |
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 13 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2604) | 1:48:A:GLN:HA | 1:48:A:GLN:HB2 | 16 | 0.1 |
| (1,2581) | 1:52:A:GLU:HA | 1:53:A:GLY:HA3 | 20 | 0.1 |
| (1,2504) | 1:138:A:GLU:HA | 1:138:A:GLU:HG3 | 13 | 0.1 |
| (1,2484) | 1:183:A:GLN:HA | 1:183:A:GLN:HB2 | 12 | 0.1 |
| (1,2479) | 1:8:A:GLN:HA | 1:8:A:GLN:HG2 | 19 | 0.1 |
| (1,2474) | 1:83:A:VAL:HA | 1:84:A:GLU:HB2 | 4 | 0.1 |
| (1,2474) | 1:83:A:VAL:HA | 1:84:A:GLU:HB2 | 14 | 0.1 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD1 | 17 | 0.1 |
| (1,2455) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HD2 | 17 | 0.1 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD1 | 17 | 0.1 |
| (1,2455) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HD2 | 17 | 0.1 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD1 | 17 | 0.1 |
| (1,2455) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HD2 | 17 | 0.1 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE1 | 1 | 0.1 |
| (1,2445) | 1:46:A:VAL:HG11 | 1:177:A:TYR:HE2 | 1 | 0.1 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE1 | 1 | 0.1 |
| (1,2445) | 1:46:A:VAL:HG12 | 1:177:A:TYR:HE2 | 1 | 0.1 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE1 | 1 | 0.1 |
| (1,2445) | 1:46:A:VAL:HG13 | 1:177:A:TYR:HE2 | 1 | 0.1 |
| (1,2444) | 1:36:A:PHE:HD1 | 1:150:A:PRO:HG2 | 17 | 0.1 |
| (1,2444) | 1:36:A:PHE:HD2 | 1:150:A:PRO:HG2 | 17 | 0.1 |
| (1,2392) | 1:31:A:PRO:HA | 1:34:A:TYR:HA | 11 | 0.1 |
| (1,2379) | 1:55:A:LYS:H | 1:55:A:LYS:HG2 | 1 | 0.1 |
| (1,2379) | 1:55:A:LYS:H | 1:55:A:LYS:HG3 | 1 | 0.1 |
| (1,2375) | 1:187:A:LYS:H | 1:187:A:LYS:HG2 | 19 | 0.1 |
| (1,2343) | 1:188:A:LYS:H | 1:188:A:LYS:HG2 | 6 | 0.1 |
| (1,2343) | 1:188:A:LYS:H | 1:188:A:LYS:HG3 | 6 | 0.1 |
| (1,2315) | 1:46:A:VAL:HG21 | 1:50:A:LEU:HG | 10 | 0.1 |
| (1,2315) | 1:46:A:VAL:HG22 | 1:50:A:LEU:HG | 10 | 0.1 |
| (1,2315) | 1:46:A:VAL:HG23 | 1:50:A:LEU:HG | 10 | 0.1 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 12 | 0.1 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 12 | 0.1 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 12 | 0.1 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG21 | 16 | 0.1 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG22 | 16 | 0.1 |
| (1,2301) | 1:100:A:THR:HA | 1:100:A:THR:HG23 | 16 | 0.1 |
| (1,2296) | 1:24:A:GLU:H | 1:58:A:LYS:HG2 | 1 | 0.1 |
| (1,2296) | 1:24:A:GLU:H | 1:58:A:LYS:HG3 | 1 | 0.1 |
| (1,2296) | 1:24:A:GLU:H | 1:58:A:LYS:HG2 | 14 | 0.1 |
| (1,2296) | 1:24:A:GLU:H | 1:58:A:LYS:HG3 | 14 | 0.1 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG21 | 2 | 0.1 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG22 | 2 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG23 | 2 | 0.1 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG21 | 17 | 0.1 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG22 | 17 | 0.1 |
| (1,2249) | 1:84:A:GLU:HA | 1:87:A:ILE:HG23 | 17 | 0.1 |
| (1,2183) | 1:28:A:PHE:HA | 1:92:A:PHE:HD1 | 18 | 0.1 |
| (1,2183) | 1:28:A:PHE:HA | 1:92:A:PHE:HD2 | 18 | 0.1 |
| (1,2052) | 1:55:A:LYS:H | 1:55:A:LYS:HD2 | 17 | 0.1 |
| (1,2052) | 1:55:A:LYS:H | 1:55:A:LYS:HD3 | 17 | 0.1 |
| (1,1999) | 1:130:A:VAL:HG11 | 1:131:A:LYS:HD3 | 13 | 0.1 |
| (1,1999) | 1:130:A:VAL:HG12 | 1:131:A:LYS:HD3 | 13 | 0.1 |
| (1,1999) | 1:130:A:VAL:HG13 | 1:131:A:LYS:HD3 | 13 | 0.1 |
| (1,1947) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HD2 | 2 | 0.1 |
| (1,1947) | 1:15:A:PRO:HB3 | 1:157:A:LYS:HD3 | 2 | 0.1 |
| (1,1916) | 1:91:A:MET:HB2 | 1:92:A:PHE:HE1 | 20 | 0.1 |
| (1,1916) | 1:91:A:MET:HB2 | 1:92:A:PHE:HE2 | 20 | 0.1 |
| (1,1879) | 1:60:A:HIS:HB3 | 1:72:A:THR:HA | 15 | 0.1 |
| (1,1825) | 1:117:A:LYS:HB3 | 1:120:A:ASP:H | 6 | 0.1 |
| (1,1799) | 1:15:A:PRO:HB2 | 1:16:A:ILE:HA | 17 | 0.1 |
| (1,1758) | 1:14:A:LYS:H | 1:14:A:LYS:HB3 | 3 | 0.1 |
| (1,1758) | 1:14:A:LYS:H | 1:14:A:LYS:HB3 | 5 | 0.1 |
| (1,1709) | 1:87:A:ILE:HG21 | 1:88:A:THR:HA | 9 | 0.1 |
| (1,1709) | 1:87:A:ILE:HG22 | 1:88:A:THR:HA | 9 | 0.1 |
| (1,1709) | 1:87:A:ILE:HG23 | 1:88:A:THR:HA | 9 | 0.1 |
| (1,1709) | 1:87:A:ILE:HG21 | 1:88:A:THR:HA | 14 | 0.1 |
| (1,1709) | 1:87:A:ILE:HG22 | 1:88:A:THR:HA | 14 | 0.1 |
| (1,1709) | 1:87:A:ILE:HG23 | 1:88:A:THR:HA | 14 | 0.1 |
| (1,1709) | 1:87:A:ILE:HG21 | 1:88:A:THR:HA | 20 | 0.1 |
| (1,1709) | 1:87:A:ILE:HG22 | 1:88:A:THR:HA | 20 | 0.1 |
| (1,1709) | 1:87:A:ILE:HG23 | 1:88:A:THR:HA | 20 | 0.1 |
| (1,1659) | 1:173:A:PHE:H | 1:176:A:GLN:HG3 | 13 | 0.1 |
| (1,1641) | 1:61:A:VAL:HG11 | 1:149:A:VAL:HB | 1 | 0.1 |
| (1,1641) | 1:61:A:VAL:HG12 | 1:149:A:VAL:HB | 1 | 0.1 |
| (1,1641) | 1:61:A:VAL:HG13 | 1:149:A:VAL:HB | 1 | 0.1 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE1 | 12 | 0.1 |
| (1,1633) | 1:37:A:GLU:HG2 | 1:92:A:PHE:HE2 | 12 | 0.1 |
| (1,1587) | 1:51:A:PRO:HA | 1:52:A:GLU:HG2 | 6 | 0.1 |
| (1,1587) | 1:51:A:PRO:HA | 1:52:A:GLU:HG3 | 6 | 0.1 |
| (1,1565) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 8 | 0.1 |
| (1,1498) | 1:107:A:ILE:HG21 | 1:111:A:PHE:HB2 | 15 | 0.1 |
| (1,1498) | 1:107:A:ILE:HG22 | 1:111:A:PHE:HB2 | 15 | 0.1 |
| (1,1498) | 1:107:A:ILE:HG23 | 1:111:A:PHE:HB2 | 15 | 0.1 |
| (1,1431) | 1:85:A:ASP:HB3 | 1:87:A:ILE:H | 10 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG11 | 14 | 0.1 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG12 | 14 | 0.1 |
| (1,1399) | 1:169:A:ASN:HB2 | 1:172:A:VAL:HG13 | 14 | 0.1 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE2 | 4 | 0.1 |
| (1,1356) | 1:11:A:THR:HG21 | 1:157:A:LYS:HE3 | 4 | 0.1 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE2 | 4 | 0.1 |
| (1,1356) | 1:11:A:THR:HG22 | 1:157:A:LYS:HE3 | 4 | 0.1 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE2 | 4 | 0.1 |
| (1,1356) | 1:11:A:THR:HG23 | 1:157:A:LYS:HE3 | 4 | 0.1 |
| (1,1354) | 1:73:A:GLN:HE22 | 1:131:A:LYS:HE2 | 10 | 0.1 |
| (1,1354) | 1:73:A:GLN:HE22 | 1:131:A:LYS:HE3 | 10 | 0.1 |
| (1,1264) | 1:29:A:TYR:HD1 | 1:64:A:LEU:HB3 | 3 | 0.1 |
| (1,1264) | 1:29:A:TYR:HD2 | 1:64:A:LEU:HB3 | 3 | 0.1 |
| (1,1264) | 1:29:A:TYR:HD1 | 1:64:A:LEU:HB3 | 6 | 0.1 |
| (1,1264) | 1:29:A:TYR:HD2 | 1:64:A:LEU:HB3 | 6 | 0.1 |
| (1,1225) | 1:163:A:GLN:HG2 | 1:164:A:GLY:H | 18 | 0.1 |
| (1,1225) | 1:163:A:GLN:HG3 | 1:164:A:GLY:H | 18 | 0.1 |
| (1,1223) | 1:161:A:ASN:HB2 | 1:164:A:GLY:H | 17 | 0.1 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 2 | 0.1 |
| (1,1170) | 1:82:A:GLY:HA3 | 1:83:A:VAL:H | 12 | 0.1 |
| (1,1154) | 1:95:A:VAL:H | 1:98:A:THR:H | 6 | 0.1 |
| (1,1141) | 1:126:A:ASN:H | 1:127:A:SER:HB3 | 17 | 0.1 |
| (1,1061) | 1:166:A:ASP:HB2 | 1:167:A:THR:H | 7 | 0.1 |
| (1,1061) | 1:166:A:ASP:HB3 | 1:167:A:THR:H | 7 | 0.1 |
| (1,1058) | 1:145:A:GLN:HE21 | 1:147:A:GLN:HA | 11 | 0.1 |
| (1,1026) | 1:67:A:LEU:H | 1:70:A:ASP:H | 2 | 0.1 |
| (1,1023) | 1:183:A:GLN:HG3 | 1:183:A:GLN:HE22 | 10 | 0.1 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 17 | 0.1 |
| (1,993) | 1:126:A:ASN:HB3 | 1:126:A:ASN:HD22 | 18 | 0.1 |
| (1,985) | 1:93:A:GLU:HB2 | 1:95:A:VAL:H | 4 | 0.1 |
| (1,985) | 1:93:A:GLU:HB3 | 1:95:A:VAL:H | 4 | 0.1 |
| (1,936) | 1:117:A:LYS:HG3 | 1:118:A:GLY:H | 2 | 0.1 |
| (1,936) | 1:117:A:LYS:HG3 | 1:118:A:GLY:H | 14 | 0.1 |
| (1,930) | 1:183:A:GLN:H | 1:184:A:LEU:HG | 15 | 0.1 |
| (1,930) | 1:183:A:GLN:H | 1:184:A:LEU:HG | 16 | 0.1 |
| (1,869) | 1:145:A:GLN:H | 1:146:A:LEU:HB2 | 14 | 0.1 |
| (1,818) | 1:105:A:ALA:HA | 1:109:A:LYS:H | 17 | 0.1 |
| (1,810) | 1:93:A:GLU:H | 1:94:A:ALA:HB1 | 17 | 0.1 |
| (1,810) | 1:93:A:GLU:H | 1:94:A:ALA:HB2 | 17 | 0.1 |
| (1,810) | 1:93:A:GLU:H | 1:94:A:ALA:HB3 | 17 | 0.1 |
| (1,788) | 1:167:A:THR:H | 1:169:A:ASN:H | 15 | 0.1 |
| (1,778) | 1:51:A:PRO:HB3 | 1:54:A:THR:H | 2 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,778) | 1:51:A:PRO:HB3 | 1:54:A:THR:H | 18 | 0.1 |
| (1,703) | 1:44:A:ASP:HB2 | 1:45:A:ASN:H | 14 | 0.1 |
| (1,703) | 1:44:A:ASP:HB3 | 1:45:A:ASN:H | 14 | 0.1 |
| (1,606) | 1:137:A:GLN:H | 1:137:A:GLN:HG2 | 10 | 0.1 |
| (1,571) | 1:50:A:LEU:H | 1:50:A:LEU:HG | 14 | 0.1 |
| (1,474) | 1:3:A:ILE:H | 1:9:A:TYR:HD1 | 4 | 0.1 |
| (1,474) | 1:3:A:ILE:H | 1:9:A:TYR:HD2 | 4 | 0.1 |
| (1,456) | 1:60:A:HIS:HB3 | 1:75:A:TRP:H | 4 | 0.1 |
| (1,456) | 1:60:A:HIS:HB3 | 1:75:A:TRP:H | 17 | 0.1 |
| (1,445) | 1:169:A:ASN:HD21 | 1:171:A:ASP:H | 9 | 0.1 |
| (1,445) | 1:169:A:ASN:HD21 | 1:171:A:ASP:H | 17 | 0.1 |
| (1,445) | 1:169:A:ASN:HD21 | 1:171:A:ASP:H | 18 | 0.1 |
| (1,445) | 1:169:A:ASN:HD21 | 1:171:A:ASP:H | 19 | 0.1 |
| (1,432) | 1:27:A:SER:H | 1:30:A:CYS:H | 7 | 0.1 |
| (1,408) | 1:2:A:GLN:H | 1:3:A:ILE:H | 6 | 0.1 |
| (1,408) | 1:2:A:GLN:H | 1:3:A:ILE:H | 8 | 0.1 |
| (1,408) | 1:2:A:GLN:H | 1:3:A:ILE:H | 12 | 0.1 |
| (1,408) | 1:2:A:GLN:H | 1:3:A:ILE:H | 19 | 0.1 |
| (1,408) | 1:2:A:GLN:H | 1:3:A:ILE:H | 20 | 0.1 |
| (1,363) | 1:112:A:VAL:HA | 1:114:A:ALA:H | 19 | 0.1 |
| (1,335) | 1:165:A:MET:HE1 | 1:166:A:ASP:H | 17 | 0.1 |
| (1,335) | 1:165:A:MET:HE2 | 1:166:A:ASP:H | 17 | 0.1 |
| (1,335) | 1:165:A:MET:HE3 | 1:166:A:ASP:H | 17 | 0.1 |
| (1,334) | 1:165:A:MET:HG2 | 1:166:A:ASP:H | 9 | 0.1 |
| (1,334) | 1:165:A:MET:HG3 | 1:166:A:ASP:H | 9 | 0.1 |
| (1,325) | 1:172:A:VAL:HG21 | 1:173:A:PHE:H | 14 | 0.1 |
| (1,325) | 1:172:A:VAL:HG22 | 1:173:A:PHE:H | 14 | 0.1 |
| (1,325) | 1:172:A:VAL:HG23 | 1:173:A:PHE:H | 14 | 0.1 |
| (1,300) | 1:130:A:VAL:HG21 | 1:131:A:LYS:H | 4 | 0.1 |
| (1,300) | 1:130:A:VAL:HG22 | 1:131:A:LYS:H | 4 | 0.1 |
| (1,300) | 1:130:A:VAL:HG23 | 1:131:A:LYS:H | 4 | 0.1 |
| (1,282) | 1:12:A:LEU:HD11 | 1:13:A:ASP:H | 1 | 0.1 |
| (1,282) | 1:12:A:LEU:HD12 | 1:13:A:ASP:H | 1 | 0.1 |
| (1,282) | 1:12:A:LEU:HD13 | 1:13:A:ASP:H | 1 | 0.1 |
| (1,281) | 1:12:A:LEU:HB2 | 1:13:A:ASP:H | 2 | 0.1 |
| (1,280) | 1:13:A:ASP:H | 1:14:A:LYS:HB2 | 4 | 0.1 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 10 | 0.1 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 10 | 0.1 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 13 | 0.1 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 13 | 0.1 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB2 | 18 | 0.1 |
| (1,272) | 1:130:A:VAL:H | 1:131:A:LYS:HB3 | 18 | 0.1 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,243) | 1:147:A:GLN:H | 1:147:A:GLN:HB3 | 11 | 0.1 |
| (1,235) | 1:87:A:ILE:HG21 | 1:89:A:ALA:H | 1 | 0.1 |
| (1,235) | 1:87:A:ILE:HG22 | 1:89:A:ALA:H | 1 | 0.1 |
| (1,235) | 1:87:A:ILE:HG23 | 1:89:A:ALA:H | 1 | 0.1 |
| (1,235) | 1:87:A:ILE:HG21 | 1:89:A:ALA:H | 18 | 0.1 |
| (1,235) | 1:87:A:ILE:HG22 | 1:89:A:ALA:H | 18 | 0.1 |
| (1,235) | 1:87:A:ILE:HG23 | 1:89:A:ALA:H | 18 | 0.1 |
| (1,223) | 1:40:A:LEU:HD11 | 1:170:A:MET:H | 6 | 0.1 |
| (1,223) | 1:40:A:LEU:HD12 | 1:170:A:MET:H | 6 | 0.1 |
| (1,223) | 1:40:A:LEU:HD13 | 1:170:A:MET:H | 6 | 0.1 |
| (1,219) | 1:34:A:TYR:H | 1:35:A:GLN:HB2 | 14 | 0.1 |
| (1,219) | 1:34:A:TYR:H | 1:35:A:GLN:HB3 | 14 | 0.1 |
| (1,201) | 1:119:A:GLU:HA | 1:121:A:TYR:H | 16 | 0.1 |
| (1,175) | 1:87:A:ILE:HG21 | 1:113:A:ASP:H | 1 | 0.1 |
| (1,175) | 1:87:A:ILE:HG22 | 1:113:A:ASP:H | 1 | 0.1 |
| (1,175) | 1:87:A:ILE:HG23 | 1:113:A:ASP:H | 1 | 0.1 |
| (1,175) | 1:87:A:ILE:HG21 | 1:113:A:ASP:H | 4 | 0.1 |
| (1,175) | 1:87:A:ILE:HG22 | 1:113:A:ASP:H | 4 | 0.1 |
| (1,175) | 1:87:A:ILE:HG23 | 1:113:A:ASP:H | 4 | 0.1 |
| (1,175) | 1:87:A:ILE:HG21 | 1:113:A:ASP:H | 12 | 0.1 |
| (1,175) | 1:87:A:ILE:HG22 | 1:113:A:ASP:H | 12 | 0.1 |
| (1,175) | 1:87:A:ILE:HG23 | 1:113:A:ASP:H | 12 | 0.1 |
| (1,175) | 1:87:A:ILE:HG21 | 1:113:A:ASP:H | 15 | 0.1 |
| (1,175) | 1:87:A:ILE:HG22 | 1:113:A:ASP:H | 15 | 0.1 |
| (1,175) | 1:87:A:ILE:HG23 | 1:113:A:ASP:H | 15 | 0.1 |
| (1,168) | 1:109:A:LYS:HA | 1:113:A:ASP:H | 17 | 0.1 |
| (1,138) | 1:80:A:ALA:H | 1:81:A:LEU:HA | 6 | 0.1 |
| (1,132) | 1:56:A:MET:HB2 | 1:57:A:THR:H | 8 | 0.1 |
| (1,42) | 1:3:A:ILE:HD11 | 1:5:A:ASP:H | 5 | 0.1 |
| (1,42) | 1:3:A:ILE:HD12 | 1:5:A:ASP:H | 5 | 0.1 |
| (1,42) | 1:3:A:ILE:HD13 | 1:5:A:ASP:H | 5 | 0.1 |
| (1,42) | 1:3:A:ILE:HD11 | 1:5:A:ASP:H | 15 | 0.1 |
| (1,42) | 1:3:A:ILE:HD12 | 1:5:A:ASP:H | 15 | 0.1 |
| (1,42) | 1:3:A:ILE:HD13 | 1:5:A:ASP:H | 15 | 0.1 |
| (1,40) | 1:5:A:ASP:H | 1:7:A:LYS:HB2 | 7 | 0.1 |
| (1,12) | 1:16:A:ILE:HD11 | 1:17:A:ALA:H | 8 | 0.1 |
| (1,12) | 1:16:A:ILE:HD12 | 1:17:A:ALA:H | 8 | 0.1 |
| (1,12) | 1:16:A:ILE:HD13 | 1:17:A:ALA:H | 8 | 0.1 |

# 10 Dihedral-angle violation analysis

No dihedral-angle restraints found